The Fermi–Pasta–Ulam problem as a challenge for the foundations of physics

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Abstract

The FPU problem is discussed in connection with its physical relevance, and it is shown how apparently there exist only two possibilities: either the FPU problem is just a curiosity, or it has a fundamental role for the foundations of physics, casting a new light on the relations between classical and quantum mechanics. To this end, a short review is given of the main conceptual proposals that have been advanced. Particular emphasis is given to the perspective of a metaequilibrium scenario, which appears to be the only possible one for the FPU paradox to survive in the physically relevant case of infinitely many particles.

Key words: FPU problem, relaxation times, metaequilibrium
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No doubt, the FPU problem (see [1] and the review [2]) did play a relevant role in the theory of dynamical systems. Indeed, first of all, with the works of Zabusky and Kruskal it prompted the modern theories of solitons and of infinitely–dimensional integrable systems. Then, it prompted the transfer of modern Hamiltonian perturbation theory to physics: we refer to KAM theory and to the subsequent weak stability theory of Nekhoroshev. However, one can very well ask what after all is the physical significance itself of the FPU problem. Here there seem to exist two extreme possibilities: 1. Just a curiosity, i.e. no physical meaning at all; 2. A fundamental meaning for the foundations of physics, in connection with the relations between classical and quantum mechanics. In the opinion of the

present authors, there is no way for intermediate possibilities concerning the physical relevance of the FPU problem. Moreover, at present, i.e. fifty years after the original FPU paper, no definitive answer allowing to decide between twe two alternatives seems to be available. The attractive feature of the present situation is that one meets here with a foundational question where little place is left for generic words, because the numerical computations of Fermi Pasta and Ulam are somehow obliging the scientific community to strive for providing a clearcut answer, which should be given by the methods of the mathematical theory of dynamical systems. The principal aim of the present paper is to explain why the physical significance of the FPU problem is bound to oscillate between such two extreme alternatives. At the same time, a short review is given of the works which were most influential in this connection.

1 Introduction: the FPU problem in the strict sense and in the wide sense, and its possible physical significance.

In its widest sense, the FPU problem may be defined as the question whether the methods of classical equilibrium statistical mechanics are justified, on a dynamical basis, in the region of very low temperatures. In a restricted sense, more akin to its original formulation, the FPU problem deals instead with an estimate of the rate of thermalization (i.e. the rate of the approach to equilibrium), if one starts out from initial data very far from equilibrium.

These are indeed old problems, but they were reopened in an acute way by the Fermi Pasta Ulam paper. In fact, the authors were reporting the results of some numerical computations for the dynamics of a discretized nonlinear string, and the results were not conforming the expectations at all. This is very well summarized in the following words, written by Ulam in a preface to the reproduction of the paper in Fermi's Collected Papers: *The results of the calculations ... were interesting and quite surprising to Fermi. He expressed to me the opinion that they really constituted a little discovery in providing intimations that the prevalent beliefs in the universality of mixing and thermalization in non–linear systems may not be always justified.* Notice that such a recollection is particularly important because the direct opinion of Fermi is not available, since he passed away before the paper was written down.

From the mathematical point of view, at first sight one might be tempted to range the FPU problem, in both of its senses (wide and restricted), within the class of problems usually dealt with by ergodic theory. But actually this is not completely true, because in ergodic theory one looks at the limit $t \to \infty$ (t being time), while here one might be dealing with situations involving metastable states (as in the case of glasses), on which nothing can be inferred from the properties holding asymptotically in time. On this point we will come back below.

But why should such rather technical problems have anything to do with the foundational problem of the relations between classical and quantum mechanics? The point is that the region of low temperatures, with which the FPU problem is concerned, is just the one where classical equilibrium statistical mechanics was confronted with its greatest qualitative failure. Indeed classical equilibrium statistical mechanics predicts a constant specific heat (i.e. one independent of temperature), while the specific heat is known to tend to zero as temperature decreases. This is actually the point where quantum mechanics made its appearence, with Planck's law taking the place of equipartition (see below). Thus the FPU result, inasmuch as it intimates *that the prevalent beliefs in the universality of mixing and thermalization in non–linear systems may not be always justified*, at first sight appears to cast doubts on the dynamical justification for using the methods of classical equilibrium statistical mechanics.

Consequently, either one is able to show that the phenomenon observed by Fermi Pasta and Ulam disappears in cases of physical interest, or one is confronted with a delicate problem of interpretation. This is the reason why the authors dealing with the FPU problem appear to be divided into two classes, according to the hopes of their hearts: 1. Those who strive for proving, on a dynamical basis, that the FPU phenomenon disappears in situations of physical interest, so that the methods of classical equlibrium statistical mechanics are applicable and classical mechanics is proven to fail, as all of us have learned at school; 2. Those who strive for proving that the methods of classical equilibrium statistical mechanics are not justified on a dynamical basis at low temperatures, so that the questions of the relations between classical and quantum mechanics should be reconsidered, in a completely new perspective. The present authors frankly recognise themselves in the second class. Most authors probably belong to the first class, although many of them may manifest sensible oscillations. In any case, such a division proved to be very effective in stimulating the mathematical research on the subject. The challenge is open.

2 The original FPU paper, and the FPU phenomenon (or paradox).

The original FPU paper was concerned with a discretized model of a string, which may also be interpreted as a one–dimensional model of a crystal. One deals with $N+2$ equal particles on a line (the extreme ones being fixed), each of the N moving particles interacting with the two adjacent ones, through a potential of the type $V(r) = (1/2)r^2 + (\alpha/3)r^3 + (\beta/4)r^4$. For $\alpha = \beta = 0$ (the unperturbed case) the system is well known to be equivalent to a system of N independent harmonic oscillators (normal modes) having certain frequencies $\omega_j = 2\sin[(j\pi)/2(N+1)]$, and so there is essentially no evolution, because the energies E_j of the normal modes are independent integrals of motion. For what concerns the perturbed system, Fermi was well acquainted with a famous theorem of Poincaré (having produced already in the year 1923 a generalization of it – see [3] or also [4]), according to which in general no integral of motion exists apart from the Hamiltonian itself, no matter how small the perturbation be. So the FPU system was expected to be ergodic. By most people this fact was interpreted as constituting a dynamical justification for the application of the methods of classical equilibrium statistical mechanics. Indeed ergodicity ensures that the time–averages of the dynamical variables converge, as $t \to \infty$, to the corresponding phase–averages, i.e. the averages with respect to Gibbs measure (we think of N large enough so that the equivalence of the various equilibrium ensembles is guaranteed). But how can such a situation be reconciled, in any reasonable continuous way, with the fact that in the unperturbed case one has an integrable system, with its N integrals of motion, somehow the opposite of an ergodic system, while ergodicity comes about no matter how small the perturbation is? Today, we know very well how continuity was restored in the measure–theoretical sense by Kolmogorov, with his formidable work of the year 1954 (the same year of the FPU work), in which the existence of individual deformed invariant surfaces was exploited (see [5]). But continuity is also restored if one makes a question of times. One should look at the *relaxation time* τ for the establishment of equilibrium, i.e. the time needed for the time–averages of relevant quantities to actually converge to the corresponding phase–averages. One expects that, as the perturbation decreases to zero, such relaxation time τ tends to infinity or, equivalently, the *thermalization rate* tends to zero. Recalling the words of Ulam quoted above, and the work of Fermi on the Poincaré theorem, one may guess that such a perspective was the one that Fermi had in mind: one should look for the time needed for equilibrium to actually be attained.

Now, the fundamental result of classical equilibrium statistical mechanics is the *equipartition theorem*: up to a small contribution vanishing with the non-linearity, all the modes should have (in phase average) the same sharing of energy, actually equal to the quantity kT, where k is the Boltzmann constant and T the absolute temperature. So what Fermi Pasta and Ulam did was to numerically integrate the equations of motion of the FPU model for initial data corresponding to a state extremely far from equipartition (the computations were done for $N = 64$ or $N = 32$ particles, with certain fixed values of α and β and also a fixed value of the energy E). In fact they chose an initial state with the energy concentrated on the lowest frequency mode $j = 1$ or on a few low–frequency modes (the *long–wavelength case*). Fermi Pasta and Ulam expected that, after a suitable time, energy would be uniformly spread among all modes, producing the flat spectrum of equipartition predicted by classical equilibrium statistical mechanics. They found instead that, up to the maximal time availabale, energy was shared only within a small packet of low–frequency modes, with no approach to equipartition at all. The key point is that one might have expected to see a progressive approach to equipartition. Instead (as vividly shown by the last figure reported in the FPU paper, which gives the time–averages $\bar{E}_j$ of the normal modes versus time) the time–averages do indeed appear to approach an equilibium, because they stabilize quite well. But such an equilibrium has nothing to do with the one predicted by classical equilibrium statistical mechanics, i.e. equipartition, because the FPU spectrum is an "anomalous" one, which has the form of an exponential decay towards the high frequencies. This fact, namely that apparently an equilibrium was reached which is however completely different from the one predicted by classical equilibrium statistical mechanics, may be called *the FPU phenomenon*, or even *the FPU paradox*.

3 The first reactions: the way out of Izrailev and Chirikov, the work of Bocchieri et al., and the proposal of Cercignani, Galgani and Scotti.

As mentioned above, the first reaction (amply quoted in the already recalled preface of Ulam) was that of Zabusky and Kruskal (see [6]). They apparently did not deal at all with the physical aspect of the paradox. They just picked up very seriously the suggestion that there exist meaningful systems which are perturbations of integrable ones and nevertheless are still integrable. Thus, they started developing the modern theories of solitons and of infinitely–dimensional integrable systems, which later took their own way, with no reference to the FPU problem at all.

A fundamental contribution in connection with the FPU paradox was soon given by Izrailev and Chirikov (see [7]). By the way, their results made such strong an impression on one of the present authors, as to lead him to study by heart, in the original russian language, a consistent part of a subsequent paper by Chirikov. The mathematical frame Izrailev and Chirikov had in mind is, as they explicitly mention, KAM theory. According to it, the perturbation of an integrable system resembles the unperturbed one, in a way which in general decreases (in a measure theoretic sense) as perturbation is increased. This naturally leads one to expect that the resemblance completely disappears above a certain threshold (often described as the transition between ordered and chaotic motions). In the present case, for α and β fixed, the quantity playing the role of the perturbation parameter is the energy E (because the cubic and quartic terms become negligible with respect to the quadratic ones, as energy tends to zero). Thus one expects that there exists an energy threshold E^c such that the FPU paradox disappears above that threshold, i.e. for $E > E^c$. And this turned out to actually be the case. Indeed, if one repeats the FPU computations for initial data of the same type as FPU, but with a large enough energy, the spectrum is found to relax, within the available time, to the flat one corresponding to equipartition. This is the Izrailev–Chirikov mechanism: equipartiton is obtained (in a short time) if energy is raised above a threshold E^c, and this certainly was a fundamental contribution.

Then comes what we like to call the *Izrailev–Chirikov conjecture*, which is a different thing, having to do with the dependence of the critical energy E^c on the number N of degrees of freedom. The conjecture is that $E^c/N \to 0$ as $N \to \infty$. More precisely, the conjecture was explicitly put forward for the case of initial data with excitations of high–frequency modes (the *short–wavelength case*), and some semianalytical considerations were also provided in order to support it. Such considerations were recently adjusted by Shepelyansky (see [8]) in order to cover the case of initial data of FPU type (the *long–wavelength case*). Denote by $\epsilon = E/N$ the specific energy of the system. If the Izrailev–Chirikov conjecture were true, then the FPU paradox would disappear for all physically relevant energies, i.e. for $\epsilon > 0$. This would be the end of the problem.

Actually, the situation turns out to be much more complicated. Indeed, the semianalytical considerations of Izrailev and Chirikov refer to the so–called criterion of the overlapping of resonances introduced by Chirikov, which, apparently, just ensures the existence of some "local chaos" (local with respect to the modes), with no direct implication for the global problem of equipartition. For what concerns the considerations of Shepelyansky, they were even interpreted quite recently (see below) as strong indications in the opposite direction, namely that the FPU phenomenon should persist in the limit $N \to \infty$. In any case, independently of its justification, the Izrailev–Chirikov conjecture may be considered as playing the role of a fundamental paradigm, namely as the suggestion that the FPU problem, even it its wide sense, be irrelevant for physics.

The subsequent main contribution came from a paper of Bocchieri, Scotti, Bearzi and Loinger (see [9]), in which numerical indications were given that the specific energy threshold E^c/N would not vanish in the limit $N \to \infty$. In fact, such authors also introduced a slight modification of the FPU model, inasmuch as the interparticle potential was chosen to be a realistic one, namely that of Lennard–Jones, $V(r) = 4V_0[(\sigma/r)^{12} - (\sigma/r)^6]$. This contains the parameters V_0 and σ, the first of which has the meaning of the depth of the potential well. The specific energy threshold could thus be given a physical interpretation, because it turned out to be of the order of $0.04\,V_0$, and this corresponds, for example in the case of Argon, to a temperature of some degrees Kelvin.

So, there could have been space for a BSBL conjecture, opposed to that of Izrailev and Chirikov, namely that the FPU problem has a physical meaning. The "*crossing of the Rubicon*" was done in a subsequent paper by Galgani and Scotti (see [10]). The main idea was that the FPU spectrum, with its exponential decay towards the high frequencies, is qualitatively of Planck's type. So a fit was made to a Planck–like law, namely $E(\omega_j) = A\omega_j/[\exp(A\beta\omega_j)-1]$, containing two parameters A (an action) and β. It was found that β depends on the specific energy as expected (namely, as an inverse temperature), while the action A appeared to be a constant. The striking fact was that, using for m (the mass of the particles), V_0 and σ the concrete values corresponding to Argon, the action A was found to be of the order of magnitude of Planck's constant $\hbar$. It took some time to understand that this had occurred just because Planck's constant had actually been introduced from outside into the model, somehow by hands, through the realistic molecular potentials. Indeed, as dimensional analysis immediately shows, any action appearing in the results has to be proportional to the natural action of the model, namely to $\sqrt{mV_0}\,\sigma$. On the other hand it is well known that, for example for the parameters of the noble gases, one has empirically the relation $\sqrt{mV_0}\,\sigma = 2Z\hbar$, where Z is the atomic number and $\hbar$ is indeed Planck's constant. After the appearing of the paper, Chirikov himself wrote a private letter to the authors, kindly asking them whether the motions involved were of an ordered or of a chaotic type, a question to which the authors were not prepared to answer. In a short time, Cercignani (see [11]) gave a further contribution "of an ideological type", by suggesting that the threshold energy should be a function $E^c(\omega)$ of the frequency (i.e. should depend on the initially excited mode, as had in fact been assumed also by Izrailev and Chirikov), and that the quantity $E^c(\omega)$ not only should not vanish in the limit $N \to \infty$, but even should be the analog of the quantum zero–point energy $(1/2)\hbar\omega$. This idea still remains in the mind of Cercignani, as one can see from the paper [12].

4 The metaequilibrium perspective.

Thus, the two extreme possibilities mentioned in the introduction had already been advanced by the year 1972: either the FPU problem is irrelevant for physics, or it has a fundamental meaning. Apparently, the decision between the two alternatives ought to be done by looking for estimates of some energy threshold distinguishing between ordered or chaotic motions. But such a mathematical scenario proved to be too naive, and a subtler one was indeed advanced.

The breakthrough was provided by a paper by Fucito et al. (see [13]), worked out in the year 1982 by a group of people around Parisi, where the new idea was introduced that the FPU phenomenon should be understood as corresponding to a situation of metaequilibrium. In other terms, the anomalous FPU spectrum should be not an equilibrium state, but rather an apparent one (a "frozen" state) which would later evolve, on a much longer time–scale, to the "true" equilibrium, i.e. to the one predicted by classical equilibrium statistical mechanics. The novelty of such an idea is that, by the ingredient of the two different time–scales, it allows to reconcile the prediction of classical equilibrium statistical mechanics, i.e. energy equipartition, (which concerns the longer time–scale) with the existence itself of the FPU phenomenon, i.e. the existence of the anomalous FPU spectrum (which is quickly formed, within the first time–scale). The idea behind what we like to call the *Izrailev and Chirikov conjecture* is that the FPU phenomenon, with its anomalous spectrum, does not occur at all for physically significant systems. Here instead the idea is that the phenomenon of the anomalous spectrum does occur, being actually reached within some short relaxation time; then it would persist, having for most purposes the appearence of a true equilibrium; but the true final equilibrium should eventually be reached only within a much longer time–scale. Concerning the apparent equilibrium, certainly the proposal of Galgani and Scotti was in the minds of the authors. Indeed the sentence which concludes the paper reads: *One of the main results is that the system approaches equilibrium with a logarithmic dependence on t, so that the nonequilibrium spectrum may persist for extremely long times, and may be mistaken for a stationary state if the observation time is not sufficiently long. It is amusing to remark that the quasi–equilibrium distribution is similar to Wien's law for black–body with a slowly varying "Planck's constant".*

For what concerns the problem of the energy threshold, here it does actually take a new form. Indeed, in the new interpretation, the existence of the FPU phenonemon requires the existence of two well separated time–scales, one leading to the metaequilibrium FPU state, the other one leading to the final equilibrium. Both of them are expected to increase as the specific energy ϵ decreases to zero (possibly, the "short" one as a power of $1/\epsilon$ – see below – , whereas the "large" one as a stretched exponential). However, above a certain threshold the two time–scales might merge, and the final equilibrium should be reached within the short time–scale.

The main idea for the analytical mechanism of the quick formation of the anomalous spectrum proposed in the paper [13] is as follows. Think of a field $\varphi(x,t)$ interpolating the discretized model, and assume it is real–analytic in x; consider also the corresponding space–Fourier transform $\hat{\varphi}(k,t)$. Then it is well known that at any time t the spectrum extends up to a characteristic wave number κ, beyond which it decays exponentially fast in k/κ. In turn, the parameter $\kappa(t)$ is essentially equal to the width of the analyticity strip about the real axis. So one has to estimate the width $\kappa(t)$ of the analiticity strip, i.e. to look for the singularities of the field and estimate their minimal distance from the real axis, as a function of time. This could be accomplished in a quite elementary way, at least for short times, in the case of a slight modification of the FPU model, namely the well known φ^4 model. Indeed, in such a model each particle, in addition to being subject to the forces of the two adjacent ones, is also attracted towards its equilibrium position by a potential proportional to the fourth power of its displacement. Thus, considering initial data of long–wavelength type (as in the FPU work), the term φ_{xx} related to the interactions of adjacent particles can be neglected (at least for short times) and one remains with an equation in which each particle moves independently of the other ones, obeying an equation of Newton type with a quartic potential, the analytical properties of which are well known. This is the way in which the singularities could be quite simply estimated analytically, for short times, in the φ^4 model, thus explaining the quick formation of a packet of low– frequency modes. Concerning the time–scale characterizing the subsequent approach to the final equilibrium, in the paper [13] only some heuristic considerations were given, based on qualitative estimates of "exit times" familiar from the theory of large deviations.

The perspective was however completely clear, and was very well illustrated in the papers [14] and [15]. In such works, numerical computations on the FPU model itself (rather than on the φ^4 model) were reported. They appeared to support, first of all, the existence of an apparent equilibrium of FPU type below a certain specific energy threshold ϵ^c, thus providing a beautiful quantitative confirmation of the previous indications of Bocchieri et al. in connection with the limit $N \to \infty$. It was however quite explicitly pointed out that such a phenomenon should be interpreted in the metastability perspective, in analogy with the phenomenology of glasses. In this connection, the result of some discussions with Parisi was summarized (see [14], page 1044) in the following terms: *The situation can be likened to the very slow relaxation behavior in disordered systems, where the evolution towards "equilibrium" takes place through metastable states approached at different time scales.* After some very interesting qualitative considerations concerning the exchanges of energy to be expected below the threshold ϵ^c *after the "frozen state" has been approached*, it was finally added: *If this were the case this energy transfer would be highly inefficient and very slow, and therefore difficult to detect numerically. In any case, the equipartition threshold observed for the integration time discussed in this paper is physically sensible when we are interested in the behavior of a system for long but finite times.*

5 An intriguing debate.

At this point, a very interesting scenario had been advanced. This allowed for the possibility of saving the FPU phenomenon, i.e. the anomalous FPU spectrum, below a certain critical specific energy ϵ^c, so that the phenomenon would survive in the limit $N \to \infty$. This was obtained by interpreting the FPU phenomenon in the metastability perspective (i.e. as a *frozen state*), thus making it compatible with the predictions of classical equilibrium statistical mechanics, which should be applicable only after a second, extremely longer, relaxation time.

The remaining open problem was then, apparently, that of confirming such a scenario, or of disproving it: certainly not an easy task, because it had been clearly stated that one would be dealing here with phenomena that are *difficult to detect numerically.* What followed was instead a much complicated phase, with an intriguing debate, about which we are not prepared to draw any clear conclusion, and in which, strangely enough, the idea of the metastabililty scenario was apparently lost (see [16], and the very interesting paper [**?**], in which a semi–analytical result for the largest Lyapunov exponent in the thermodynamic limit was given).

The only comment we, the present authors, can safely make is that the perspective advanced by Parisi was not really fully understood by us. Indeed, in the meantime we happened to be fully immersed in a related quite difficult and interesting problem. This was mostly concerned with the "final" extremely slow approach to equilibrium, looked at in the perspective of Nekhoroshev theorem (see [17]), or of the "Landau–Teller method", rather than with the existence of intermediate *frozen* states. The discussion of this point would require a long digression on the analog of the FPU problem for polyatomic molecules (see for example [18] and [19]), on which we do not enter here.

The metastability perspective did actually reemerge in the FPU problem after it had been rediscoveved in the framework of the studies on the specific heat (see the next section), and, later on, in some recent studies on the FPU problem itself (see [20]). A relevant contribution in this direction also came from two recent analytical works which shed some light on the quick formation of the metastable "frozen" state. We refer to the works of Ponno and Bambusi (see [21], and the paper [22] appearing in this issue). In such papers, the mechanism of Fucito et al. explaining, in the φ^4 model, the short–time formation of a packet involving low–frequency modes with an exponential tail towards the high frequencies, is reinterpreted in a way which allows to extend it to the FPU problem itself (for a previous attempt, see [23]), and moreover has the beautiful feature of building up a bridge with the original works of Zabusky and Kruskal. The very simple idea is that one should look at the analytical properties of suitable PDE's (such as the familiar KdV equation, which is suited for long–wavelength initial data). Indeed, along the lines of Zabusky and Kruskal, such PDE's are shown to provide approximations (i.e suitable normal forms) for the FPU model which are good *up to a short time*, increasing as an inverse power of the perturbation. In such a way, through the analyticity properties of such PDEs, the analyticity properties of the FPU model too are estimated, for times short enough as the ones involved in the FPU phenomenon.

Notice furthermore that the work of Shepelyansky mentioned above was also reconsidered in this perspective (see [24]). It was thus shown that the analytical considerations of Shepelyansky do actually appear to bring support to the persistence of the FPU phenomenon in the limit $N \to \infty$, inasmuch as all the available estimates turn out to be functions of the energy E only through the specific energy $\epsilon = E/N$.

Coming finally to the problem of applying the methods of perturbation theory in the limit $N \to \infty$, which is the one of interest for the FPU problem, one should mention that one meets here with a great difficulty, because the available formulation of the theory loses sense in that limit (see for example [25]). A preliminary step forward was made in the papers [26]. But a consistent approach which be able to combine the methods of perturbation theory with those of probabilility theory, to the effect that very improbable situations are excluded, is still lacking. Fortunately enough, such a difficulty seems to have now been overcome. Indeed, just in these days it has been possible (see [27]) to implement a few steps of perturbation theory in the limit $N \to \infty$ in a probabilistic frame. This was actually performed for a model which is physically significant though analytically simpler than the FPU one (the so called model of rotators). One may hope that such results can be extended to any order of perturbation theory (so that estimates of Nekhoroshev type could be obtained), for quite generic models. This would allow to obtain estimates of an exponential type for the relaxation–time to the "final" equilibrium, by a method somehow complementary to that of Parisi.

6 The FPU problem in the wide sense: the problem of the specific heats.

Sometimes it occurs that, in a field of research, a relevant step forward which a posteriori might even appear trivial, takes instead a long time to be made. In the case of the FPU model the relevant step involved two features, namely: 1. To look at quantities having a physical interest; 2. To make predictions for initial data of generic type, i.e. extracted from a Gibb's distribution at a certain temperature. Here, the main quantity of physical interest certainly is the specific heat as a function of temperature; indeed, as recalled above, it should be constant (apart from a small contribution due to the nonlinearity) according to classical equilibrium statistical mechanics, while it should tend to zero for vanishing temperatures according to the phenomenology (the third principle of thermodynamics), in agreement with quantum equilibrium statistical mechanics.

The merit of doing such a step forward, i.e. of producing estimates for the specific heat in the FPU model for generic initial data, goes to Livi, Pettini, Ruffo and Vulpiani, with their work [28] of the year 1987. Their conclusion was that the FPU model predicts a specific heat in complete agreement with classical equilibrium statistical mechanics, but it will be discussed below how the correct conclusion, at least for the one–dimensional case $d = 1$, may rather be the opposite one.

The way in which they proceeded was completely far from trivial, because their reasoning actually had a noble antecedent, although they might be unaware of that. We refer to the celebrated *dreimänner Arbeit*, namely the work of Born, Heisenberg and Jordan [29] of the year 1926. The main idea behind that celebrated paper was to study the energy fluctuations of a small piece of a string. As the computers were not yet available, and computations had to be made by hand, the attention was restricted to the integrable case, namely the linear one (which corresponds to the unperturbed case of the FPU model). The physical relevance in the present case is that the energy fluctuations of a piece of the chain *might* (see below) be expected to provide an estimate of the specific heat of that piece, because of the familiar relation between energy fluctuations and spercific heat which holds in the Gibb's ensemble.

In the paper [28] the analogous computations were made for the actual nonlinear FPU model, by evaluating the dynamical fluctuations of the energy of a piece of the chain, through numerical solutions of the corresponding equations of motion. The initial data were of generic type, i.e. were extracted from a Gibbs distribution at a given inverse temperature β, i.e. at a given specific energy $\epsilon \simeq 1/\beta$, with β in a certain range. The specific heat thus estimated turned out to be in complete agreement with the equilibrium fluctuation formula, i.e. to be constant (apart from a small contribution due to the nonlinearity) as a function of temperature. The key point is that this occurred in the whole range of temperatures explored, notwithstanding the fact that the corresponding range of specific energies contained the critical specific energy ϵ^c, which, according to a series of other numerical computations, had been estimated as characterizing the threshold between equipartition and nonequipartition in the FPU problem in the restricted sense (with initial data very far from equilibrium). In more explicit terms: the possible energy threshold of the standard FPU problem appeared to have no relevance for the specific heat.

The next step was made in a series of papers by a group of people around Tenenbaum (see [30]). The general approach was in principle the same as that of Livi et al. The relevant difference was however the choice of the subsystem, of which the energy fluctuations should be calculated. Indeed, the subsystem was not a spatially localized one, i.e. a piece of the discretized string, but rather a subset of normal modes, typically a packet of normal modes with frequencies in a certain range $(\bar{\omega}, \bar{\omega}+\Delta\omega)$. The specific heat was then estimated as in the paper [28], with reference however to the energy fluctuations of the given packet of modes. The computations were performed for the FPU model in dimension $d = 3$, with realistic Lennard–Jones potentials, and the specific heat thus estimated appeared to decrease from the "classical value" to zero, as temperature decreases. No systematic study was however made of the dependence of the results on the observation time.

The situation thus seemed to be rather paradoxical, and it was not at all clear how one could possibly reconcile such a striking difference in the results. It is the opinion of the present authors that actually no one of the above two procedures for estimating the specific heat is completely justified, although the second one might perhaps be in a better position. It was eventually understood that a more sound basis for estimating the specific heat in terms of dynamical energy fluctuations should be found in the fluctuation–dissipation theorem, as will be described below.

A first step in this direction was to eliminate at all the problem of which type of subsystem should be chosen, and this was done by making reference to the way in which the specific heat measurements are actually performed. Indeed, in the actual thermometric measurements there is no subsystem at all. The whole system in study is put in contact with a calorimeter, and the quantity which is actually considered is the energy exchanged between the whole system in study and the calorimeter, the exchange being measured through the temperature change of the calorimeter.

So a new model was considered (see [31]), in which the familiar one–dimensional FPU system is put in interaction with a a calorimeter. The latter was modeled by a perfect gas, each molecule of which could exchange energy with one extreme particle of the FPU system through collisions involving a molecular potential. In turn, the temperature of the calorimeter was defined in the familiar mechanical way through the mean kinetic energy of its molecules. In such a way it was found that the specific heat appears to decrease as temperature decreases. More precisely, here too a systematic study of the dependence of the results on the observation time was lacking. But now this occurred by an explicit choice. Indeed the numerical experiment was conceived as simulating what in the phenomenology of glasses is called a *cooling process* (or, analogously, a *heating process*), namely a process in which the temperature of the calorimeter is changed by a fixed quantity after a fixed time step. In such a work, by the way, it was strongly emphasized that the behaviour of the FPU system actually presents a strong analogy with that of glasses. In fact, as was mentioned above, this analogy had been previously suggested by Parisi but was later somehow forgotten.

Eventually, the specific heat of a FPU system was indeed estimated just in these days (see [32]), by making reference to the relation between specific heat and energy fluctuations provided by the fluctuation–dissipation theorem. One considers a FPU system, with initial data extracted from a Gibb's distribution at a given inverse temperature β, the system being in contact with a heat reservoir (modeled as above) at the *same* inverse temperature β. The energy E of the FPU system then changes with time, as does the energy (heat) exchanged with the calorimeter, and the measured specific heat C_β too. According to the fluctuation–dissipation theorem, the specific heat is estimated in terms of the energy fluctuations through the formula $C_\beta(t) = (1/2)\beta^2 < [E(t) - E(0)]^2 >_\beta$, where $< \cdot >_\beta$ denotes average with respect to the initial data, extracted according to the given Gibb's measure. In the numerical computations it is found, first of all, that the quantity $C_\beta(t)$ does indeed relax (within a relaxation time τ which increases as temperature decreases) to some final value, which thus provides the estimated value of the specific heat "after the measurement has terminated". For large temperatures the estimated value turns out to agree very well with the one predicted by classical equilibrium statistical mechanics, while for lower temperatures the "final" value is sensibly lower. Apparently, this should be a manifestation of the fact that a metastable state shows up in the specific heat problem too, because a subsequent appoach to the "really final" equilibrium value is expected. On the other hand, it is clesr that an experimenter measuring the specific heat would interpret the apparent stabilization of the quantity $C(t)$ after the first relaxation time as if it corresponded to a true equilibrium. In such a way it may be said that a phenomenon analogous to that of the standard FPU paradox has been observed also in connection with the specific heat problem. Analogous computations for dimension $d = 2$ or $d = 3$ are still lacking.

7 Conclusions

Wec hope we have convinced the reader that the FPU problem, in both of it senses, the strict one (rate of approach to equilibrium for initial data very far from equilibrium) and the wide, physically more relevant, one (specific heat as a function of temperature), is still open.

It should be made clear however that, today, apparently no one doubts that the dynamics should agree with the predictions of classical equilibrium statistical mechanics in the limit $t \to \infty$. Indeed it was illustrated above how, with respect to the years 60's, the perspective has now changed, reference being made not to KAM theory but rather to the metastability scenario, somehow analogous to that of the phenomenology of glasses. At sufficiently low temperatures, there would exist at least two relaxation times: a first relaxation process would quickly lead to a metaequilibrium ("frozen") state, whereas the subsequent approach to the final equilibrium would take an extremely longer time. Only the latter state, which is usually described in a loose way as occurring in the limit $t \to \infty$, would correspond to a standard Gibb's equilibrium, whereas the statistics dynamically consistent with the metaequilibrium state might be a different one. Thus one would be confronted with the hard question of principle of finding a generalization of statistical thermodynamics suited to metaequilibrium states. For a recent progress see [33].

In the future it should be decided whether such a metastability scenario is correct or not, particularly in the physically relevant case of dimension $d = 3$, about which very little is known at present (see however the quite interesting results [34] obtained in these days by Benettin for $d = 2$). If such a scenario proved to be correct, the main consequence would be that at low temperatures the methods of classical equilibrium statistical mechanics would not be justified on a dynamical basis, for finite extremely long times. For example, the specific heat corresponding to the metaequilibrium state might to all practical purposes be qualitatively similar to that predicted by quantum equlibrium statistical mechanics. In such a case it is obvious that at least the minimalistic consequence should be accepted that the relations between classical and quantum mechanics should be reconsidered in a completely new perspective. Some hints in this direction, inspired by old papers of Einstein and Nernst, have been advanced (see [35]).

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