Dynamical Systems and Thermodynamics

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Introduction

The relations between thermodynamics and dynamics are dealt with by statistical mechanics. For a given dynamical system of Hamiltonian type in a classical framework, it is usually assumed that a dynamical foundation for equilibrium statistical mechanics, namely for the use of the familiar Gibbs ensembles, is guaranteed if one can prove that the system is ergodic, i.e. has no integrals of motion apart from the Hamiltonian itself. One of the main consequences is then that classical mechanics fails in explaining thermodynamics at low temperatures (we are thinking of the specific heats of crystals or of polyatomic molecules, or of the related black–body problem), because the classical equilibrium ensembles lead to equipartition of energy for a system of weakly coupled oscillators, against the third principle. This is actually the problem that historically led to the birth of quantum mechanics, equipartition being replaced by Planck's law. At a given temperature T, the mean energy of an oscillator of angular frequency ω is not $k_B T$ (with k_B the Boltzmann constant), and thus is not independent of frequency (equipartition), but decreases to zero exponentially fast as frequency increases.

Thus, the problem of a dynamical foundation for classical statistical mechanics would be reduced to ascertaining whether the Hamiltonian systems of physical interest are ergodic or not. It is just in this spirit that many mathematical works were recently addressed at proving ergodicity for systems of hard spheres, or more generally for systems which are expected to be not only ergodic but even hyperbolic. However, a new perspective was opened in the year 1955, with the celebrated paper of Fermi, Pasta and Ulam, which constituted the last scientific work of Fermi.

The FPU paper was concerned with numerical computations on a system of N (actually, 32 or 64) equal particles on a line, each interacting with the two adjacent ones through nonlinear springs, certain boundary conditions having being assigned (fixed ends). The model mimicks a one dimensional crystal (or also a string), and can be described in the familiar way as a perturbation of a system of N normal modes, which diagonalize the corresponding linearized system. The initial conditions corresponded to the excitation of only a few low–frequency modes, and it was expected that energy would rather

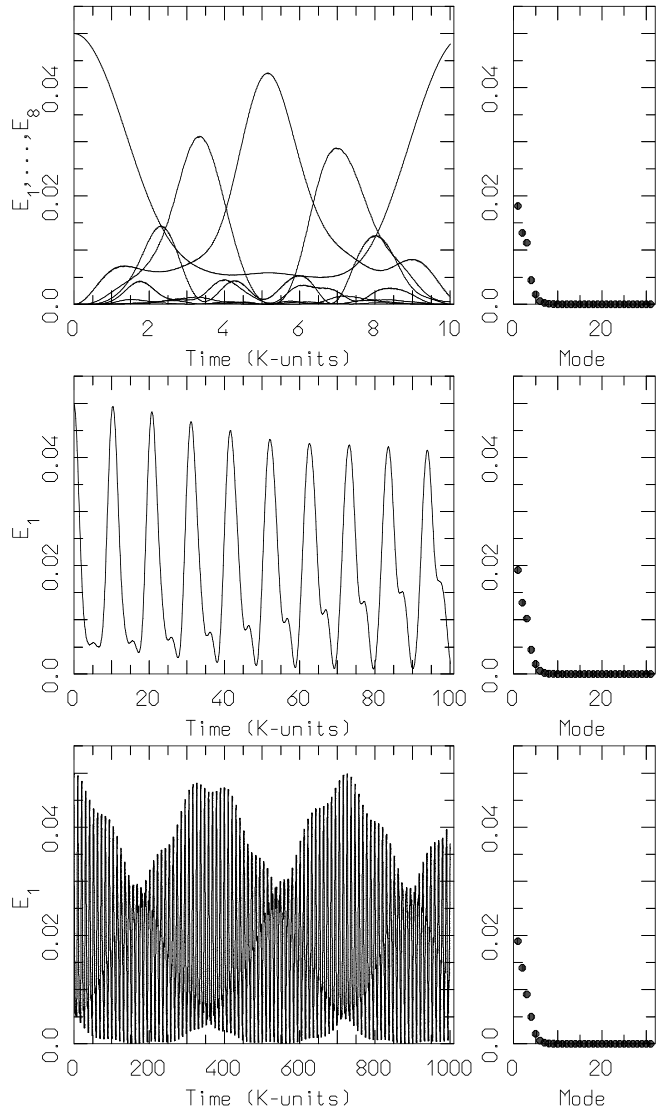

FIG. 1: The FPU paradox: normal mode energies E_j versus time (left) and energy spectrum, namely time–average of E_j versus j, (right) for three different time–scales. The energy, initially given to the lowest–frequency mode, does not flow to the high–frequency modes within the accessible observation time. Here, $N = 32$.

quickly flow to the high–frequency modes, thus estab-

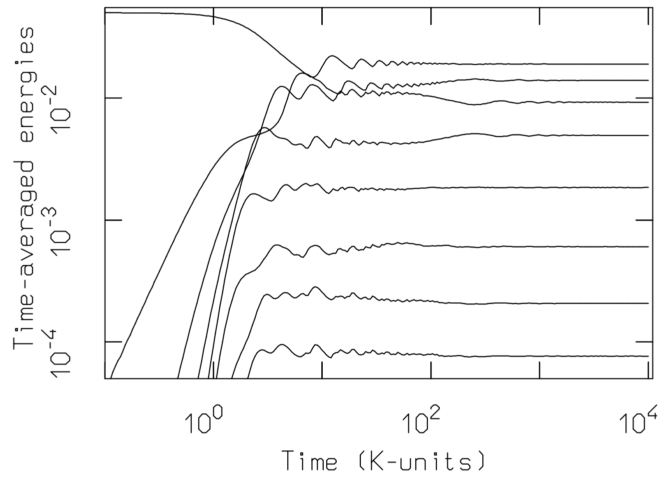

FIG. 2: The FPU paradox: time–averages of the mode energies versus time for the same run as Fig. 1. The spectrum has reached an apparent equilibrium, different from that of equipartition predicted by classical equilibrium statistical mechanics. An exponential decay of the tail is clearly exhibited.

lishing equipartition of energy, in agreement with the predictions of classical equilibrium statistical mechanics. But this did not occur within the available computation times, and the energy rather appeared to remain confined within a packet of low–frequency modes having a certain width, as if being in a state of apparent equilibrium of a non standard type. This fact can be called "*the FPU paradox*". In the words of Ulam, written as a comment in Fermi's Collected Papers, this is described as follows: "*The results of the computations were interesting and quite surprising to Fermi. He expressed the opinion that they really constituted a little discovery in providing intimations that the prevalent beliefs in the universality of mixing and thermalization in nonlinear systems may not be always justified.*"

The FPU paper had immediately a very strong impact in the theory of dynamical systems, because it motivated all the modern theory of infinite–dimensional integrable systems and solitons (KdV equation), starting from the works of Zabusky and Kruskal (1965). But in such a way the FPU paradox was somehow enhanced, because the FPU system turned out to be associated to the class of integrable systems, namely the systems having a number of integrals of motion equal to the number of degrees of freedom, which are in a sense the most antithermodynamic systems. The merit of establishing a bridge towards ergodicity goes to Izrailev and Chirikov (1966). Making reference to the most advanced results then available in the perturbation theory for nearly–integrable systems (KAM theory), those authors pointed out that ergodicity, and thus equipartition, would be recovered if one took initial data with a sufficiently large energy. And this was actually found to be the case. Moreover, it turned out that their work, and its subsequent completion by Shepelyanski, were often interpreted as supporting the conjecture that the FPU paradox would disappear in the thermodynamic limit (infinitely many particles, with finite density and energy density). The opposite conjecture was advanced in the year 1970 by Bocchieri, Scotti, Bearzi and Loinger, and its relevance for the relations between classical and quantum mechanics was immediately pointed out by Cercignani, Galgani and Scotti. A long debate then followed. Possibly, some misunderstandings occurred, because in the discussions concerning the dynamical aspects of the problem reference was generally made to notions involving infinite times. In fact, it had not yet been conceived that the FPU equilibrium might actually be an apparent one, corresponding to a sort of intermediate metaequilibrium state. This was for the first time suggested by a group of people around Parisi in the year 1982. The analogy of such a situation with those occurring in glasses was pointed out more recently.

In the present article the state of the art of the FPU problem is discussed. The thesis of the present authors is that the FPU phenomenon survives in the thermodynamic limit, in the last mentioned sense, namely in the sense that at sufficiently low temperatures there exists a kind of metaequilibrium state surviving for extremely long times. The corresponding thermodynamics turns out to be different from the standard one predicted by the equilibrium ensembles, inasmuch as it presents qualitatively some quantum–like features (typically, specific heats in agreement with Nernst's third principle). The key point, with respect to equilibrium statistical mechanics, is that the internal thermodynamic energy should be identified not with the whole mechanical energy, but only with a suitable fraction of it, to be identified through its dynamical properties, as was suggested more that a century ago by Boltzmann himself, and later by Nernst.

Here, it is first discussed why nearly–integrable systems can be expected to present the FPU phenomenon. Then the latter is illustrated. Finally, some hints are given for the corresponding thermodynamics.

Nearly–integrable versus hyperbolic systems, and the question of the rates of thermalization

As mentioned above, it is usually assumed that the problem of providing a dynamical foundation to classical statistical mechanics is reduced to the mathematical problem of ascertaining whether the Hamiltonian systems of physical interest are ergodic or not. However, there remains open a subtler problem. Indeed, the notion of ergodicity involves the limit of an infinite time (time averages should converge to ensemble averages as $t \to \infty$), while intermediate times might be relevant. In this connection it is convenient to distinguish between two classes of dynamical systems, namely the hyperbolic and the nearly–integrable ones.

The first class, in a sense the prototype of chaotic systems, should include the systems of hard spheres (very much studied after the classical works of Sinai), or more generally the systems of mass–points with mutual repulsive interactions. For such systems it can be expected that the time–averages of the relevant dynamical quantities in an extremely short time converge to the corresponding ensemble averages, so that the classical equilibrium ensembles could be safely used.

A completely different situation occurs for the dynamical systems such as the FPU one, which are nearly–integrable, i.e., are perturbations of systems having a number of integrals of motion equal to the number of degrees of freedom. Indeed, in such a case ergodicity means that the addition of an interaction, no matter how small, makes an integrable system lose all of its integrals of motion, apart from the Hamiltonian itself. And in fact this quite remarkable property was already proven to be generic by Poincaré, through a set of considerations which had a fundamental impact on the theory of dynamical systems itself. In view of its importance for the foundations of statistical mechanics, the proof given by Poincaré was reconsidered by Fermi, who added a subtle contribution concerning the role of single invariant surfaces. It is just to such a paper that Ulam makes reference in his comment to the FPU work mentioned above, when he says: "*Fermi's earlier interest in the ergodic theory is one motive*" for the FPU work.

The point is that the picture which looks at the ergodicity induced on an integrable system by the addition of a perturbation, no matter how small, somehow lacks continuity. One might expect that, in situations in which the nonlinear interaction which destroys the integrals of motion is very small (i.e. at low temperatures), the underlying integrable structure should somehow be still appreciable, in some continuous way. In fact, continuity should be recovered by making a question of times, namely by considering *the rates of thermalization* (to use the very FPU words), or equivalently the *relaxation times*, namely the times needed for the time–averages of the relevant dynamical quantities to converge to the corresponding ensemble averages. By continuity, one clearly expects that the relaxation times diverge as the perturbation tends to zero. But more complicated situations might occur, as for example the existence of two (or more) relevant time–scales. The point of view that time–scales of different orders of magnitude might occur in dynamical systems (with the exhibition of an interesting example) and that this might be relevant for statistical mechanics, was discussed by Poincaré himself in the year 1906.

The FPU phenomenon: historical and conceptual developments

We now illustrate the FPU phenomenon, following essentially its historical development. We will make reference to Figs. 1–8, which are the results of numerical integrations of the FPU dynamical system. If $x_1, \cdots, x_N$ denote positions of the particles (of unitary mass), or more precisely the displacements from their equilibrium positions), and p_i denote the corresponding momenta, the Hamiltonian is

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N+1} V(r_i) \ ,$$

where $r_i = x_i - x_{i-1}$ and one has taken a potential $V(r) = r^2/2 + \alpha r^3/3 + \beta r^4/4$ depending on two positive parameters α and β. Boundary conditions with fixed ends, namely $x_0 = x_{N+1} = 0$, are considered. We recall that the angular frequencies of the corresponding normal modes are $\omega_j = 2\sin[j\pi/2(N+1)]$, with $j = 1, \cdots, N$; it is thus convenient to take as time unit the value π, which is essentially, for any N, the period of the fastest normal mode.

The original FPU result is illustrated in Figs. 1 and 2. Here $N = 32$, $\alpha = \beta = 1/4$, and the total energy is $E = 0.05$; the energy was given initially to the first normal mode (with vanishing potential energy). Three time–scales (increasing from top to bottom) are considered, the top one corresponding to the time–scale of the original FPU paper. In the left boxes the energies $E_j(t)$ of modes j are reported versus time ($j = 1, \cdots, 8$ at top, $j = 1$ at center and bottom). In the right boxes we report the corresponding spectra, namely the time–average (up to the respective final times) of the energy of mode j versus j, for $1 \le j \le N$. In Fig. 2 we report, for the same run of Fig. 1, the time–averages of the energies of the various modes versus time; this figure corresponds to the last one of the original FPU work. The facts to be noticed in connection with these two figures are the following ones: 1) the spectrum (namely the distribution of energy among the modes, in time average) appears to have relaxed very quickly to some form, which remains essentially unchanged up to the maximum observed time; 2) there is no global equipartition, but only a partial one, because the energy remains confined within a group of low–frequency modes, which form a small packet of a certain definite width; 3) the time evolutions of the mode energies appears to be of quasiperiodic type, since longer and longer quasi–periods can be observed as the total time increases.

After the works of Zabusky and Kruskal, by which the FPU system was somehow assimilated to an integrable system, the bridge toward ergodicity was made by Izrailev and Chirikov (1966), through the idea that there should exist a stochasticity threshold. Making reference to KAM theory, which had just been formulated in the frame of perturbation theory for nearly–integrable systems, their main remark was the following one. It is known that KAM theory, which essentially guarantees a behavior similar to that of an integrable system, applies only if the perturbation is smaller than a certain threshold; on the other hand, in the FPU model the natural perturbation parameter is the energy E of the system. Thus the FPU phenomenon can be expected to disappear above a certain threshold energy E_c. This is indeed the case, as illustrated in Figs. 3 and 4. The parameters α, β and the class initial data are as in Fig. 1. In Fig. 3 the total time is kept fixed (at 10000 units), whereas the energy E is increased in passing from top to bottom, actually 0.1 to $E = 1$ and $E = 10$. One sees that at $E = 10$ equipartition is attained within the given observation time; correspondingly, the motion of

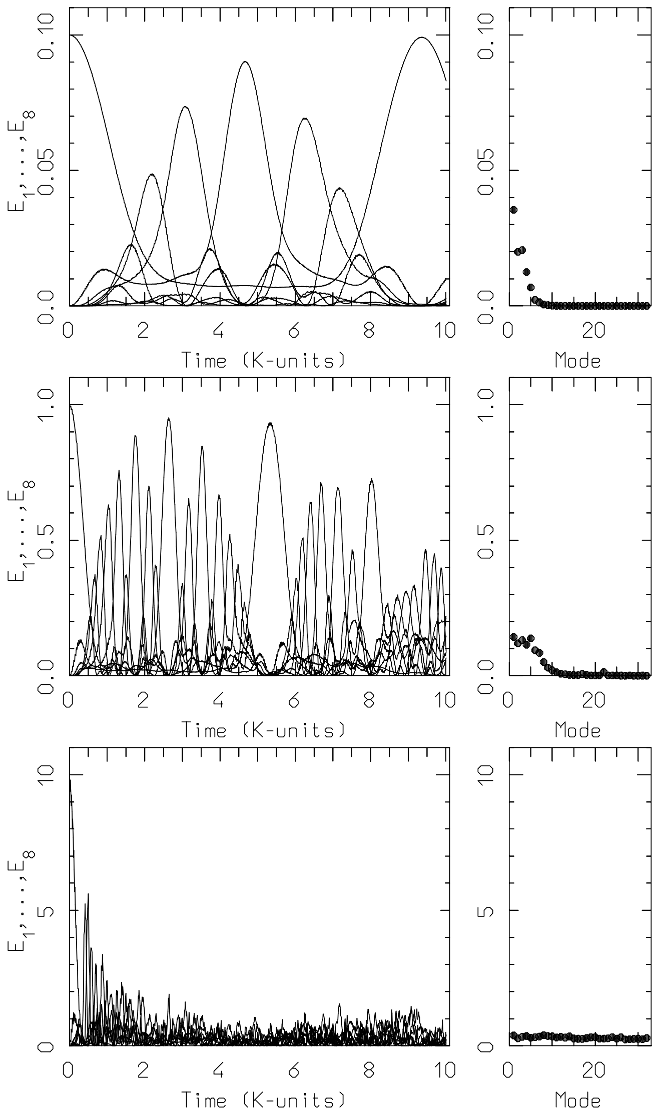

FIG. 3: The Izrailev–Chirikov contribution: for a fixed observation time, equipartition is attained if the initial energy E is high enough. Here, from top to bottom, $E = 0.1,\ 1,\ 10$.

the modes visually appears to be nonregular. The approach to equipartition at $E = 10$ is clearly exhibited in Fig. 4, where the time–averages of the energies are reported versus time.

There naturally arose the problem of the dependence of the threshold E_c on the number N of degrees of freedom (and also on the class of initial data). Certain semianalytical considerations of Izrailev and Chirikov were generally interpreted as suggesting that the threshold should vanish in the thermodynamic limit for initial excitations of high–frequency modes. Recently Shepelyanski completed their analysis by showing that the threshold should vanish also for initial excitations of the low–frequency modes, as in the original FPU work (see however the subsequent paper by Ponno mentioned below). If this were true, the FPU phenomenon would disappear in the thermodynamic limit. In particular, the equipartition principle

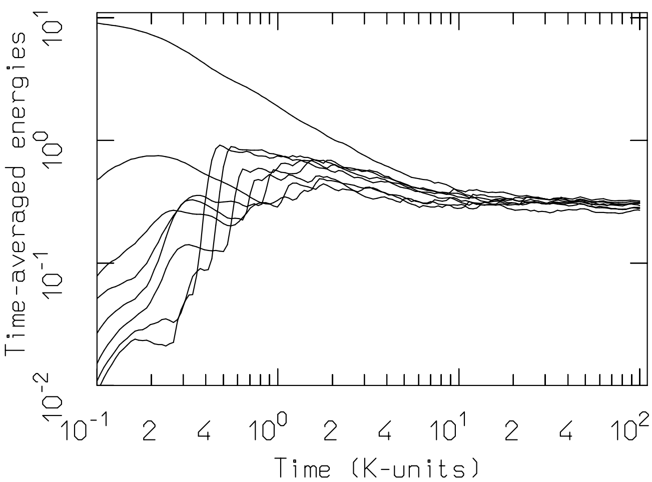

FIG. 4: The Izrailev–Chirikov contribution: time–averages of the mode energies versus time for the same run as at bottom of Fig. 3.

would be dynamically justified at all temperatures.

The opposite conjecture was advanced by Bocchieri, Scotti, Bearzi and Loinger (1970). This was based on numerical calculations, which indicated that the energy threshold should be proportional to N, namely that the FPU phenomenon persists in the themodynamic limit provided the specific energy $\epsilon = E/N$ is below a critical value ϵ_c, which should be definitely nonvanishing. Actually, the computations were performed on a slightly different model, in which nearby particles were interacting through a more physical Lennard–Jones potential. By taking concrete values having a physical significance, namely the values commonly assumed for Argon, for the threshold of the specific energy they found the value $\epsilon_c \simeq 0.04\,V_0$, where V_0 is the depth of the Lennard–Jones potential well. This corresponds to a critical temperature of the order of some degrees Kelvin. The relevance of such a conjecture (persistence of the FPU phenomenon in the thermodynamic limit) was soon strongly emphasized by Cercignani, Galgani and Scotti, who also tried to establish a connection between the FPU spectrum and Planck's distribution.

Up to this point the discussion was concerned with the alternative whether the FPU system is ergodic or not, and thus reference was made to properties holding in the limit $t \to \infty$. Correspondingly, one was making reference to KAM theory, namely to the possible existence of surfaces (N-dimensional tori) which should be dynamically invariant (for all times). The first paper in which the attention was drawn to the problem of estimating the relaxation times to equilibrium is the one by Fucito et al. (1982). The model considered was actually a different one (the so called φ^4 model), but the results can be extended to the FPU model too. Analytical and numerical indications were given for the existence of two time-scales. In a short time the system was found to relax to a state characterized by a FPU–like spectrum, with a plateau at the low frequencies, followed by an exponential tail. This however appeared as being a sort of metastable state. In their words: "*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*". Indeed, on a second much larger time–scale the slope of the exponential tail was found to increase logarithmically with time, with a rate which decreases to zero with the energy. This is an indication that the time for equipartition should increase as an exponential with the inverse of the energy.

This is indeed the picture that the present authors consider to be essentially correct, being supported by very recent numerical computations, and by analytical considerations. Curiously enough, however, such a picture was not fully appreciated until quite recently. Possibly, the reason is that the scientific community had to wait until becoming acquainted with two relevant aspects of the theory of dynamical systems, namely Nekhoroshev theory and the relations between KdV equation and resonant normal form theory.

The first step was the passage from KAM theory to Nekhoroshev theory. Let us recall that, while in KAM theory one looks for surfaces which are invariant (for all times), in Nekhoroshev theory one looks instead for a kind of weak stability involving finite times, albeit "extremely long" ones, as they are found to increase as stretched exponentials with the inverse of the perturbative parameter. Thus one meets with situations in which one can have instability over infinite times, while having a kind of practical stability up to exponentially long times. Notice that Nekhoroshev's theory was formulated only in the year 1974, and that it started to be known in the west only in the early years 80's, just because of its interest for the FPU problem. Another interesting point is that just in those years one started to become acquainted with a related historical fact. Indeed, the idea that equipartition might require extremely long times, so that one would be confronted with situations of a practical lack of equipartition, has in fact a long tradition in statistical mechanics, going back to Boltzmann and Jeans, and later (in connection with sound dispersion in gases of polyatomic molecules) to Landau and Teller.

In such a way the idea of the existence of extremely long relaxation times to equipartition came to be accepted. The ingredient that was still lacking is the idea of a quick relaxation to a metastable state. The importance of this should not be overlooked. Indeed, without it one cannot at all have a thermodynamics different from the standard equilibrium one corresponding to equipartition. This was repeatedly emphasized, against Jeans, by Poincaré on general grounds and by Nernst on empirical grounds. The full appreciation of this latter ingredient was obtained quite recently (although it had been clearly stated in the quoted paper of Fucito et al.). A first hint in this direction came from the realization (see Fig. 5) of a deep analogy between the FPU phenomenon and the phenomenology of glasses. Then there came a strong numerical indication by Berchialla, Galgani and Giorgilli. Finally, from the analytical point of view, there was a suitable revisitation (by Ponno) of the traditional connection between the FPU system and the KdV equation with its solitons. The relevant points are the following ones: 1) the KdV equation describes well the solutions of the FPU problem (for initial data of FPU type) only on a "short" time–scale, which increases as a power of $1/\epsilon$, and so describes only a first process of quick relaxation; 2) the corresponding spectrum has a well definite analytical form, the energy being spread up to a maximal frequency $\bar{\omega}(\epsilon) \simeq \epsilon^{1/4}$ and then dacaying exponentially ; 3) the relevant formulæ contain the energy only through the specific energy ϵ, and thus can be expected to hold also in the thermodynamic limit. It should be mentioned however that all the results of an analytic type mentioned above have a purely formal character, because up to now no one of them was proven, in the thermodynamic limit, in the sense of rigorous perturbation theory. This requires a suitable readaptation of the known techniques, which is being obtained in the present days both in connection with Nekhoroshev's theorem (in order to explain the extreme slowness of a possible final approach to equilibrium) and in connection with the normal form theory for partial differential equations (in order to explain the fast relaxation to the metaequilibrium state).

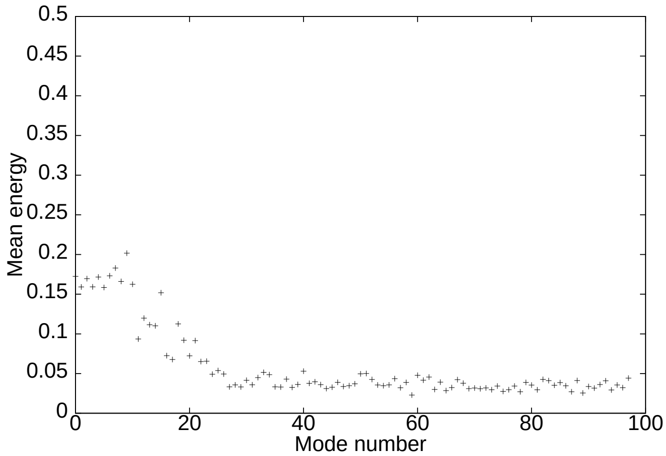

FIG. 5: Analogy with glasses: the specific energy u of an FPU system is plotted versus temperature T for a cooling process (upper curve) and a heating process (lower curve), the FPU system being in contact with a heat reservoir, whose temperature is changed at a given rate. At low temperatures the system does not time to reach the equilibrium curve $u = T$ (with $k_B = 1$). From A. Carati, L. Galgani *Journ. Stat. Phys.* **94**, 859 (1999).

In conclusion, the situation seems to be the following one, for the case of initial conditions of the FPU type (excitation of a few low–frequency modes). The first phenomenon that occurs in a "short" time (of the order of $(1/\epsilon)^{3/4}$ is a quick relaxation to the formation of what can be called a *natural packet* of low–frequency modes extending up to a certain maximal frequency $\bar{\omega} \simeq \epsilon^{1/4}$.

This is a phenomenon which has nothing to do with any diffusion in phase space. In fact, it shows up also for an integrable system such as a Toda lattice (as will be illustrated below), and should be described by a suitable resonant normal form related to the KdV equation. One has then to take into account the fact that the domain of the frequencies in the FPU model is bounded ($\omega < 2$ in the chosen units). Now, as the function $\bar{\omega}(\epsilon)$ is monotonous, this fact leads to the existence of a critical value ϵ_c of the specific energy ϵ, defined by $\bar{\omega}(\epsilon_c) = 2$. Indeed, for $\epsilon > \epsilon_c$ the quick relaxation process leads altogether to equipartition. Below threshold, instead, the same quick process leads to the formation of a FPU–like spectrum, involving only modes of sufficiently low frequency. This should however be a metastable state (which might be mistaken for a stationary one), that should be followed, on a second time–scale, by a relaxation to the final equilibrium, through a sort of Arnold diffusion requiring extremely long Nekhoroshev–like times. This is actually the way in which the old idea of a threshold, originally conceived in terms of KAM tori, is now recovered even for ergodic systems, in terms of time–scales.

The existence of a process of quick relaxation, and of a threshold in the above mentioned sense, is illustrated in Figs. 6 and 7. In Fig. 6 the lower part refers to the FPU model, while the upper one refers to a corresponding Toda model. The latter is in a sense the prototype of an integrable nonlinear system; with respect to the FPU case, the difference is that the potential $V(r)$ is now exponential. The parameters of the exponential were chosen so that the two models coincide up to cubic terms in the potential. With the energy given to the lowest–frequency mode, the figure shows how much time is needed in order that energy spreads up to a mode $\bar{k}$, for several values of $\bar{k}$, as a function of ϵ. It is seen that in the Toda model (top) there is formed a packet extending up to rather well defined width, and that this occurs within a relaxation time increasing as a power of $1/\epsilon$. An analogous phenomenon occurs for the FPU model (bottom). The only difference is that, below a critical specific energy $\epsilon_c \simeq 0.1$, there exists a subsequent relaxation time to equipartition, which involves a time growing faster than any inverse power of ϵ. Such a second phenomenon is due to the nonintegrable character of the FPU model. In the next Fig. 7 the width of the natural packet for the FPU model is exhibited, by reporting the frequency $\bar{\omega}$ of its highest mode as a function of ϵ. As one sees, the numerical results clearly indicate the existence of a relation $\bar{\omega} \simeq \epsilon^{1/4}$, which holds for a number of degrees of freedom N ranging from 8 to 1023. This is actually the law which is predicted by resonant normal form theory.

Boltzmann and Nernst revisited

All the results illustrated above were referring to initial data of FPU type, namely with an excitation of a few low–frequency modes. However, from the point of view of statistical mechanics such initial data are exceptional, and one should rather consider initial data extracted from the Gibbs distribution at a certain temperature. One can

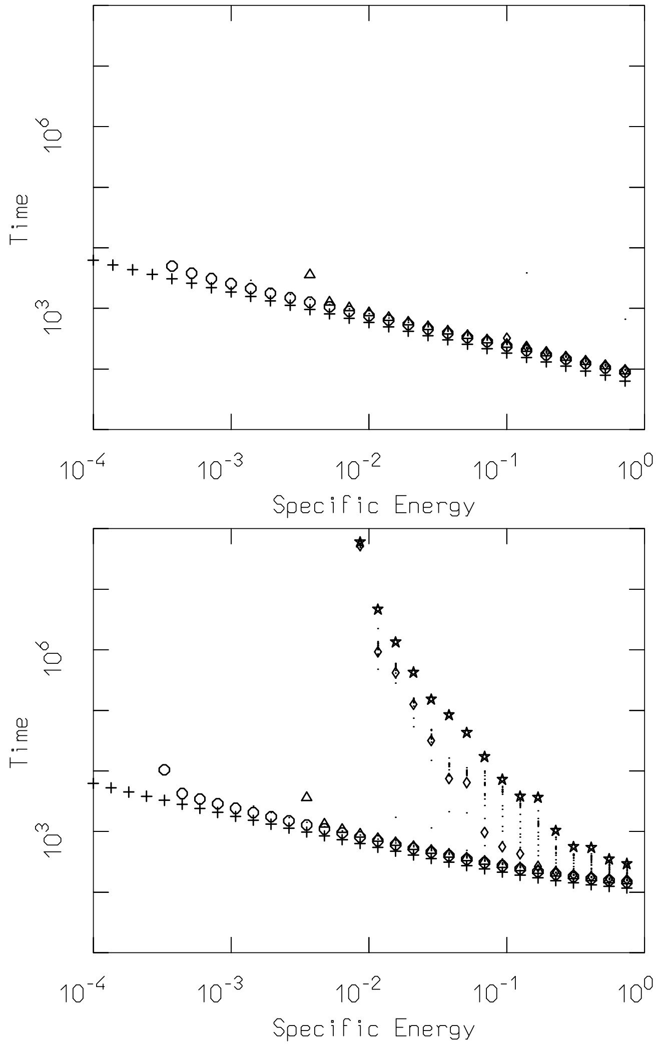

FIG. 6: Time needed to form a packet versus specific energy for the FPU model (bottom) and the corresponding Toda model (top). Different symbols refer to packets of different width. The existence of two times–scales below a critical specific energy in the FPU model is exhibited. For more details see L. Berchialla, L. Galgani, A. Giorgilli, *Discr. Cont. Dyn. Systems* **B** (2004), in press.

then couple the FPU system to a heat bath at a slightly different temperature, and look at the spectrum of the FPU system after a certain time. The result, for the case of a heat bath at a higher temperature, is shown in Fig. 8. Clearly one has here a situation similar to that occurring for initial data of FPU type, because only a packet of low–frequency modes exhibits a reaction, each of its modes actually adapting itself to the temperature of the bath, whereas the high–frequency modes do not react at all, i.e. remain essentially frozen.

This capability of reacting to external disturbances (which seems to pertain only to a fraction of the mechanical energy initially inserted into the system) can be characterized in a quantitative way through an estimate of the fluctuations of the total energy of the FPU system.

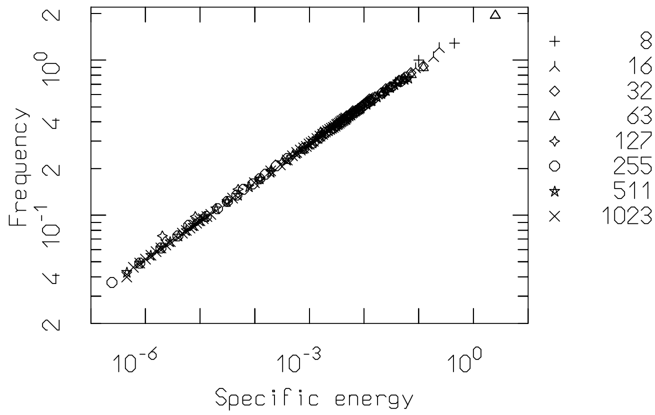

FIG. 7: Width of the natural packet versus specific energy, for N ranging from 8 to 1023. From L. Berchialla, L. Galgani, A. Giorgilli: *Discr. Cont. Dyn. Systems* **B** (2004), in press.

This is indeed the sense of the fluctuation–dissipation theorem, the precursor of which is perhaps the contribution of Einstein to the first Solvay Conference (1911). Through such a method, the specific heat of the FPU system is estimated (apart from a numerical factor) by the time average of $[E(t) - E(0)]^2$, where $E(t)$ is the energy, at time t, of the FPU system in dynamical contact with a heat bath (at the same temperature from which the initial data are extracted). Usually, in the spirit of ergodic theory one looks at the infinite–time limit of such a quantity. But in the spirit of the metastable picture described above, one can check whether the time–average presents a previous stabilization to some value smaller than the one predicted at equilibrium. Such a result, which is in qualitative agreement with the third principle, has indeed obtained (by Carati) in these days.

In conclusion, in situations of metaequilibrium such as

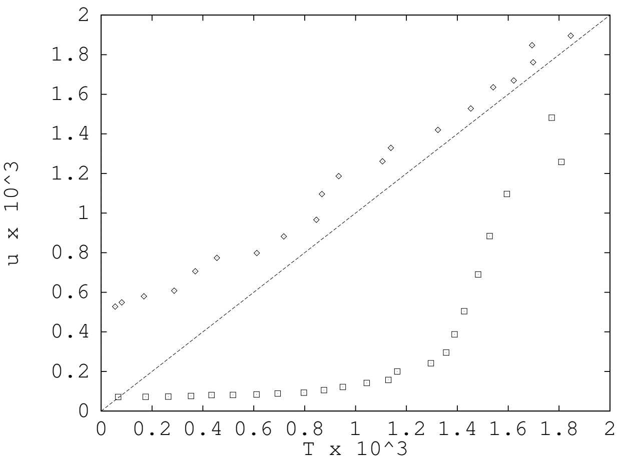

FIG. 8: A case of an FPU system initially at equilibrium and thus in equipartition. Spectrum of the FPU system after having been in contact with a heath reservoir at a higher temperature. From A. Carati, P. Cipriani, L. Galgani, *Journ. Stat. Phys.* **115**, 1119 (2004).

those existing in the FPU model at low temperatures, a thermodynamics can still be formulated. Indeed, just in virtue of the quick relaxation process described above, the time–averages of the relevant quantities are found to stabilize in rather short times. In such a way one overcomes the critique of Poincaré to Jeans, namely that one cannot have a thermodynamics at all if reference is made only to the existence of extremely long relaxation times to equilibrium. The difference with respect to the standard equilibrium thermodynamics relies now in the mechanical interpretation of the first principle. Indeed the internal thermodynamic energy is identified not with the whole mechanical energy, but just with that fraction of it which is capable of reacting in short times to the external perturbations.

This is the way in which the old idea of Boltzmann (and Jeans) might perhaps be presently implemented. For what concerns the fraction of the mechanical energy which is not included in the thermodynamic internal energy, as not being able to react in relatively short times, this should somehow play the role of a zero–point energy. This was suggested in the year 1971 by C. Cercignani. But in fact, such a conception was put forward by Nernst himself in an extremely speculative work of the year 1916. In such a work Nernst also advanced the conception that, for a system of oscillators of a given frequency, there should exist both dynamically ordered (*geordnete*) and dynamically chaotic (*ungeordnete*) motions, the latter ones being prevalent above a certain energy threshold. According to him, this fact should be relevant for a dynamical understanding of the third principle and of Planck's law.

Everyone knows that the modern theory of dynamical systems made people become acquainted with the (sometimes abused) notions of order and chaos and of a transition between them. One might say that the FPU work just forced the scientific community to take into account such notions in connection with the principle of equipartition of energy. It is really moving to see that the same notions, with the same words, had already been introduced much before on purely thermodynamic grounds, in connection with the relations between classical and quantum mechanics.

See also

Statistical mechanics. Quantum statistical mechanics; introductory article. Ergodic theory. Perturbations of integrable Hamiltonian systems. Stability theory/KAM. Theory of weakly coupled oscillators. Introductioon to integrable systems. Soliton equations. Toda lattices.

Further Reading

E. Fermi, J. Pasta, S. Ulam, in E. Fermi, Collected Papers, University of Chicago Press (Chicago, 1965): see

N. 266 and N. 11.
N.J. Zabusky, M.D. Kruskal, Phys. Rev. Lett. **15**, 240 (1965).
F.M, Izrailev, B.V. Chirikov, Sov. Phys. Dokl. **11**, 30 (1966); D.I. Shepelyansky, Nonlinearity **10**, 1331 (1997); A. Ponno, Europh. Lett. **64**, 606 (2003).
L. Galgani, A. Scotti, Rivista Nuovo Cim. **2**, 189–209 (1972).
E. Fucito, F. Marchesoni, E. Marinari, G. Parisi, L. Peliti, S. Ruffo, A. Vulpiani, Journal de Physique **43**, 707–713 (1982).
G. Benettin, L. Galgani, A. Giorgilli, Nature **311**, 444 (1984).
L. Boltzmann, Nature **51**, 413 (1895); Lectures on Gas Theory, University of California Press (Berkeley, 1964), Vol. II, Sects. 43–45 ; W. Nernst, Verh. Dtsch. Phys. Ges. **18**, 83 (1916); H. Poincaré, J. de Phys. Th. Appl. **5**, 369 (1906).

Keywords

KAM theory, Nekhoroshev theory, integrable systems, nearly-integrable systems, ergodic theory, Gibbs ensembles, internal energy, solitons, energy equipartition, Planck's law, third principle.