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On the Definition of Temperature in FPU Systems

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It is usually assumed, in classical statistical mechanics, that the temperature should coincide, apart from a suitable constant factor, with the mean kinetic energy of the particles. We show that this is not the case for Fermi–Pasta–Ulam systems, in conditions in which energy equipartition between the modes is not attained. We find that the temperature should be rather identified with the mean value of the energy of the low frequency modes.

KEY WORDS: FPU; specific heat; nonequilibrium; glasses.

1. INTRODUCTION

The Fermi–Pasta–Ulam system consists of a chain of N nonlinear oscillators with certain given boundary conditions, tipically fixed ends. It is well known (see refs. 1 and 2) that, for energies below a certain threshold E_c, if the energy is initially given to a few low frequency modes, equipartition of energy among the modes is eventually attained only after an extremely long time, while at intermediate times a kind of metaequilibrium state is attained, in which the energy is shared essentially within a packet of low frequency modes.

An interesting and much discussed problem, is whether the specific energy threshold E_c/N vanishes or not in the limit of an infinite number of particles. Here we leave this problem aside: we will suppose for example that the number N of particles be fixed, so that the threshold certainly exists. We address instead the problem raised by the fact that below the threshold one meets, as in the theory of glasses, with time scales to thermal equilibrium which are very long, even longer than any fixed observational

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time scale. Does this lack of thermalization have any consequences on the relevant thermodynamical quantities? or even, is it possible to correctly (i.e., uniquely) define the quantities of interest? In other words, is it still possible to have a thermodynamics below the threshold?

In the literature, the discussion is usually focused on the specific heat, because from heuristic arguments it is suggested that to less chaotic motions there correspond smaller specific heats, with eventually zero specific heat for totally ordered motions (i.e., for integrable systems). Thus it is expected that by lowering the energy below threshold the specific heat should diminish; such a property, in turn, should be considered as a good indicator of the weakening of chaos.

The papers,(3, 4) which aim at evaluating the specific heat of Fermi–Pasta–Ulam systems below threshold by numerical computations, reach two opposite conclusions: in ref. 3 the value of the specific heat remains constant (as would follow from the equipartition principle) even below the threshold, while in ref. 4 the specific heat indeed begins to fall down, below the threshold, and finally vanishes as temperature goes to zero. This striking difference is apparently due to the different methods used in the two papers in estimating the specific heat. Actually, in both papers the Fermi–Pasta–Ulam system is kept isolated (fixed ends), so that a direct measurement of the specific heat is precluded (because a direct measurement requires at least one heat bath). The specific heat is then estimated from the fluctuations of energy of a subsystem through the well known relation between specific heat and mean square deviation of energy, which holds in the canonical ensemble. The two papers differ in the choice of the subsytem: in the paper,(3) one considers the energy fluctuations of a small piece of the total chain, while in ref. 4 one considers the energy fluctuations of a small packet of nearby modes. As the energy of each mode remains nearly constant below the threshold while the energy of a piece of chains still presents large fluctuations, this indeed explains why the two papers reach opposite conclusions. Now, at most only one of the conclusions can be correct, if a right conclusion does exist at all; indeed it is not clear whether the specific heat can be defined in an unambiguous way below the threshold.

A different approach was proposed in the paper.(5) In short, the basic remark is the following one. As the above mentioned relation between specific heat and energy fluctuations is obtained from the equilibrium Gibbs ensemble, then its validity below the threshold is in doubt just because, up to the considered times, the system has not yet thermalized. So, it is argued that in measuring the specific heat one should revert to the conventional method which makes use of a heat bath at a given temperature T coupled to the Fermi–Pasta–Ulam system, with the corresponding familiar calorimetric expression for the specific heat. Namely, the energy exchange ΔQ between the bath and the Fermi–Pasta–Ulam system is measured when the temperature is varied by ΔT, then the ratio $\Delta Q/\Delta T$ is computed, and (in principle) the limit is taken for vanishing ΔT. However, even with such a method, one is still confronted with a delicate problem, because the amount of exchanged energy ΔQ does depend on how much time one has waited in making the measurement (this is the so-called waiting time problem of the theory of glasses). The curve predicted by equipartition is recovered for infinitely long waiting times, while for finite waiting times the specific heat is expected to vanish at sufficiently low temperatures.

The question is thus: does there exist a natural way to choose a definite waiting time? Another problem then arises, due to the fact that, in the ratio $\Delta Q/\Delta T$ defining the specific heat, one should insert in the denominator the variation of temperature of the Fermi–Pasta–Ulam system and not that of the bath. The question is then whether the temperature of the Fermi–Pasta–Ulam system is the same as that of the heat bath. The very fact that the quantity ΔQ depends on the waiting time actually shows that this is not the case, just because the equality of the two temperatures would imply $\Delta Q = 0$. On the other hand, if one were able to identify the temperature of the Fermi–Pasta–Ulam system, then the question of the waiting time would have a quick answer: one should wait until the heat bath temperature and that of the Fermi–Pasta–Ulam system have become equal, and only at that time should one measure the corresponding energy exchange. So the possibility of having available well defined thermodynamic quantities on short time scales is based on the possibility of providing a good notion of temperature for the FPU system before complete equipartition be achieved. From this point of view, the identification usually made of the temperature of the Fermi–Pasta–Ulam system with the mean kinetic energy of its particles is not the correct one, because in such a case the temperatures of the two systems (Fermi–Pasta–Ulam system and heat bath) would remain different for extremely long times.

The identification of the mean kinetic energy with temperature is so deeply rooted in our minds, that the existence of another quantity playing that role seems hardly conceivable. The aim of this paper is to show instead that this is possible.

In Section 2 we give a preliminary discussion of the zeroth law for states of metaequilibrium such as those of the Fermi–Pasta–Ulam system below threshold, in Section 3 we describe the model we employ for measuring of the temperature of the Fermi–Pasta–Ulam system through heat baths by numerical computations, and the numerical results are given in Section 4. Some final comments are given in Section 5; in particular, a comparison is made of the present model with other ones also involving chains coupled to heat baths.

2. ZEROTH LAW AND TEMPERATURE IN STATES OF METAEQUILIBRIUM

One of the basic features of thermal equilibrium is the so-called zeroth law, which essentially amounts to the transitivity of the equilibrium. From this follows (see ref. 6) that for any system there exists a function of its macroscopic state (the so called *empirical temperature*) which has the same value for bodies in equilibrium.

However, it is not granted that, for a given macroscopic state, the equilibrium is unique if some of the internal degrees of freedom are dynamically frozen. We are thinking typically of the case of polyatomic molecules (see ref. 8) for which it is known that the exchanges of energy between the center of mass and the internal degrees of freedom are so slow that the number of effective degrees of freedom depends on the time of observation. This is actually the general situation that occurs in states of metaequilibrium.

We thus address the problem whether it is possible to have a zeroth principle, and so also an empirical temperature, in situations of metaequilibrium, in which the physical quantities are changing only on a very long time scale. So, if we put our Fermi–Pasta–Ulam system in heat contact with another body, and observe that at first there is a rapid relaxation to a certain state, while a later evolution to a final equilibrium would take place on a time scale much longer than our observational scale, we can think of our system as if it were equilibrated. Obviously, one is not granted that in such a situation the zeroth law, i.e., the transitivity of this metaequilibrium state, holds. But, if this is the case, an empirical temperature can be defined. In other terms, if we put the Fermi–Pasta–Ulam system in contact with a thermometer which, after a short transient, appears to have reached a temperature T (not evolving on our time scale), and if later, after having put the Fermi–Pasta–Ulam system in contact with another body (for example a heat bath) at the same temperature T, nothing seems to occur (i.e., there is no exchange of energy in mean between the bodies), then the metastable state reached does have the transitive property, and we are authorized to assign to the Fermi–Pasta–Ulam system the temperature T reached by the thermometer.

An equivalent arrangement, which we have actually implemented in our numerical simulations to be described below, is the following one: the Fermi–Pasta–Ulam system is put at the same time in contact both with a heat bath and with a thermometer (obviously, with no direct connection between the two external bodies). In such a situation, the transitive property reduces to the property that in a short time the thermometer attains the same temperature of the heath bath; the subsequent evolution to a final equilibrium should take place later, at a much smaller rate. Then, *by definition*, the temperature of the Fermi–Pasta–Ulam system in the metaequilibrium state is the one reached by the thermometer after the short-time relaxation.

This definition can appear satisfactory from an operative point of view. However, as it stands, it still lacks a clear connection with the properties of the Fermi–Pasta–Ulam system itself. Indeed there remains the problem of understanding, how the zeroth law can hold even if the Fermi–Pasta–Ulam system did not yet thermalize. In this connection, we make reference to a known phenomenon(2) concerning the isolated Fermi–Pasta–Ulam system, namely the fact that, below threshold, for initial excitations of the low frequency modes the energy turns out to remain confined to modes below a certain critical mode k_{cr}, while the higher modes are not significantly involved in the dynamics. Notice, moreover, that an analogous phenomenon, i.e., a dynamical involvement restricted to the modes of sufficiently low frequency, is know to occur also when a system is coupled to an external body, for the case of polyatomic molecules (see ref. 7). So, it is known that, on a short time scale, the high frequencies modes (above k_{cr}) do not get dynamically involved, neither by the internal nonlinarities nor by an interaction with external bodies. In both cases a packet of low frequency modes is formed which are in mutual equilibrium, and moreover are active in the process of thermalization with external bodies. Only after a much larger time scale there follows a relaxation of the Fermi–Pasta–Ulam system to the true equilibrium state. Before, it appears as if there existed an adiabatic partition (of a dynamical nature) between low and high frequency modes.

If this is the correct picture, it is clear to what property of the Fermi–Pasta–Ulam system should our definition of temperature correspond: namely, to the mean energy of each of the low frequency modes (those below k_{cr}). In the rest of the paper we will illustrate the results of some numerical computations, which, in our opinion, strongly support the fact that such a metaequilibrium is transitive, and that the empirical temperature thus defined coincides with the energy of the low frequency modes.

3. THE MODEL

As mentioned above, the model is constituted by a Fermi–Pasta–Ulam system in contact with two bodies, acting, the one as a thermometer and the other one as a heat bath. We make the simplest choice, in which the two bodies are perfect gases. Each gas is modeled as a system of point particles having no interactions among them, while interacting with the Fermi–Pasta–Ulam system through some smooth force between each of the gas particles and one of the edge Fermi–Pasta–Ulam particles. In more detail, concerning the Fermi–Pasta–Ulam system we denote as usual by x_i, $i=1,\dots,N$, the distance of the ith particle from its equilibrium position, by p_i its conjugate momentum, and consider the familiar "β-model" Hamiltonian

$$H_{\mathrm{FPU}}=\sum_{i=1}^{N}\frac{p_i^2}{2m}+\sum_{i=0}^{N}\left[\frac{\Omega^2}{2}(x_{i+1}-x_i)^2+\frac{\beta}{4}(x_{i+1}-x_i)^4\right], \tag{1}$$

involving two positive parameters β and Ω, with fixed boundary conditions $x_0=0$, $x_{N+1}=0$. Now, to the "left" of the Fermi–Pasta–Ulam chain we place a perfect gas which acts as a heat bath: denoting by y_i, π_i the ith gas particle's position and momentum respectively, we have $-L<y_i<x_1$, with $L>0$ playing the role of the volume of the gas. The motion of each particle is thus free apart from the fact that it suffers an elastic reflection as $y_i=-L$, and that it moreover interacts with the first Fermi–Pasta–Ulam particle x_1 through a short range potential, which we choose as

$$V=V_0\,\frac{e^{-(y_i-x_1)/l_0}}{(y_i-x_1)/l_0},$$

l_0 and V_0 denoting its range and strength respectively. In agreement with the bound given above, due to the singularity of the potential at $y_i=x_1$, the solutions $y_i(t)$ of the equations of motion cannot cross the point $x_1(t)$, i.e., for all times t one has $-L<y_i(t)<x_1(t)$. The Hamiltonian of the heat bath is thus

$$H_{\mathrm{B}}=\sum_{i=1}^{N}\left[\frac{\pi_i^2}{2m}+V_0 l_0\,\frac{e^{-(y_i-x_1)/l_0}}{(y_i-x_1)}\right], \tag{2}$$

supplemented by the boundary condition that the particles are reflected at $y_i=L$.

To the "right" of the Fermi–Pasta–Ulam chain we place the thermometer, which is taken again as a perfect gas, with Hamiltonian

$$H_{\mathrm{T}}=\sum_{i=1}^{N}\left[\frac{\tilde{\pi}_i^2}{2m}+V_0 l_0\,\frac{e^{-(\tilde{y}_i-x_N)/l_0}}{(\tilde{y}_i-x_N)}\right], \tag{3}$$

(plus a reflection condition at $\tilde{y}_i=L$) where $\tilde{y}_i$, $\tilde{\pi}_i$ are the positions and momenta of the gas particles respectively; each of the particles interacts only with the last particle x_N of the Fermi–Pasta–Ulam system via the same potential as for the heath bath.

In our simulations we chose an equal number of particles for the three systems, while in principle the number of bath particles should be larger than that of the Fermi–Pasta–Ulam system, and this in turn should be larger than that of the thermometer. Our choice is dictated only by the computational power available: we cannot take the total number of particles too large, but at the same time the number of particles in each system cannot be too small if a good statistics has to be insured. Taking the same number $N = 100$ of particles for each of the three subsystems, seemed to us a good compromise.

We took as units of mass, length and energy the values m, l_0, and V_0, which were thus put equal to one in our computations. The values of the parameters Ω and β were set equal to $\Omega = 400$ and $\beta = 3742$ respectively. Such strange values come from the following consideration: the intermolecular interaction in a crystal is well represented by a Lennard-Jones potential, whose relevant parameters (the range and the strength) are of order one with our choice of units. On the other hand the Fermi–Pasta–Ulam potential should just be a Taylor expansion of the Lennard-Jones potential around the equilibrium position. Performing such a Taylor expansion and putting the parameters equal to one, the indicated values for Ω and β are found.

Finally in our numerical simulations we took $L = 25$; this in order to ensure a sufficient total number of collisions (of the order 10^6 in our actual integrations), while at the same time letting the gas particles be free for a large part of their paths.

4. NUMERICAL RESULTS

The integration step was taken equal to a twentieth of the shortest period $\tau_{\mathrm{f}} = \pi/\Omega$ of the Fermi–Pasta–Ulam chain, and the numerical solutions were computed up to times of order $2 \cdot 10^7 \tau_{\mathrm{f}}$.

The numerical experiments were performed in the following way. For the bath we chose a temperature T_1 and took random initial conditions extracted from a Maxwellian at the chosen temperature T_1 (we also checked that the value of the mean kinetic energy should not deviate too much from the expected one, in order to avoid too large fluctuations); for the Fermi–Pasta–Ulam system we chose initial data at equipartition with a temperature $T_1/10$ and random phases; finally for the thermometer we chose initial data in the same way as for the heath bath, but at a temperature $T_1/10$. We let the system evolve for a time $10^4 \tau_{\mathrm{f}}$, and then began to compute the time averages of the kinetic energies of the gases and of the harmonic energy of the Fermi–Pasta–Ulam system. The results of the computations for two representative cases are shown in Figs. 1 and 2, where we report, versus time, the temperatures (i.e., twice the kinetic energies per particle) of the gases and the harmonic energy per particle of the Fermi–Pasta–Ulam system (actually, time averages of such quantities are reported). Let us recall that such three quantities should be equal according to the equipartition principle, i.e., for sufficiently long times.

In Fig. 1, we started with a temperature $T_1 = 1$. One sees that, after a time of order $10^5 \tau_f$, the temperatures of two gases and the specific harmonic energy of the Fermi–Pasta–Ulam system have become essentially equal, although still presenting significant fluctuations. This case should correspond to a situation of thermal equilibrium.

Figure 2 refers instead to the choice of $T_1 = 0.4$. One sees that the heat bath and the thermometer still reach the same temperature (although after a time almost one order of magnitude larger than before), while the specific harmonic energy per particle of the Fermi–Pasta–Ulam system remains well below the common temperature of the two gases, up to the observation time. Actually the curve is so flat that the Fermi–Pasta–Ulam system can be expected to possibly reach the equilibrium only on a totally different

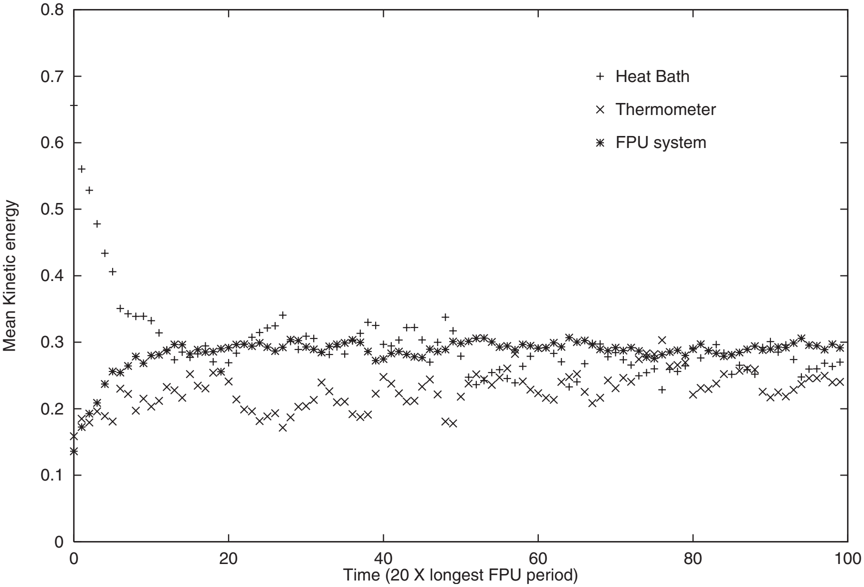

Fig. 1. Specific harmonic energy of the FPU system, and twice the specific energies of the gases, versus time, at high temperature.

time scale. The global system seems indeed to be in a situation of metaequilibrium.

It appears, however, that the zeroth law can still be valid, and that the temperature "measured" by the thermometer is a good empirical one, because the temperatures of the two gases have become equal. To understand to which quantity of the Fermi–Pasta–Ulam system does this measured temperature correspond, in Figs. 3 and 4 we report the spectra (time-averaged energies of the modes versus mode number) of the Fermi–Pasta–Ulam system at the end of the two runs. Figure 3 refers to the case of complete thermalization, and correspondingly a complete equipartition among the modes is found, as expected. More interesting is Fig. 4: here equipartition obtains only among modes of sufficiently low frequency, say below $k_{\mathrm{cr}} = 10$, while the energy starts decreasing for larger values of k, going down, say for $k > 25$, to the initial equipartition value 0.04. It does not appear as a surprise to observe that the mean energy of the low frequency modes essentially agrees with the common temperature of the two gases. This seems to indicate that, for our metastable state, the "good" definition of temperature of the Fermi–Pasta–Ulam system is the mean energy of the (sufficiently) low frequency modes.

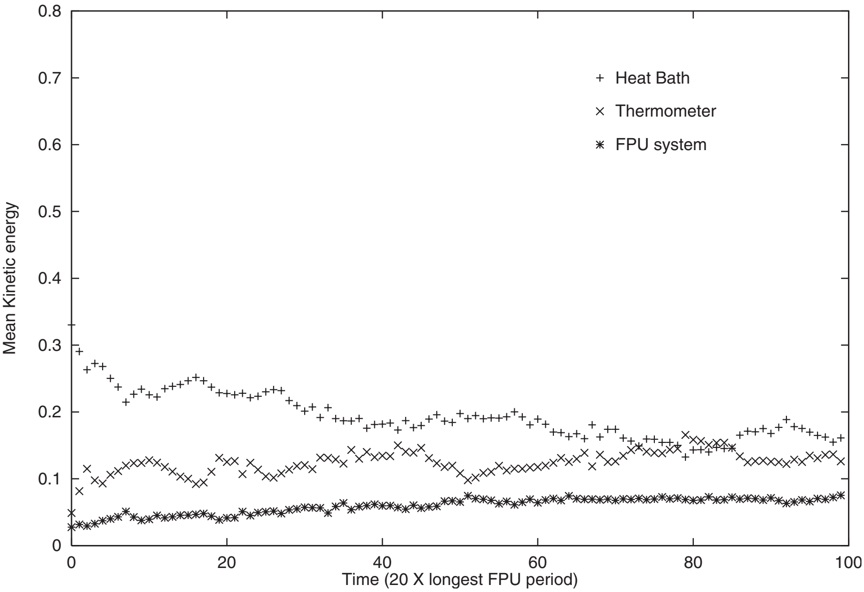

Fig. 2. Same as Fig. 1, at low temperature.

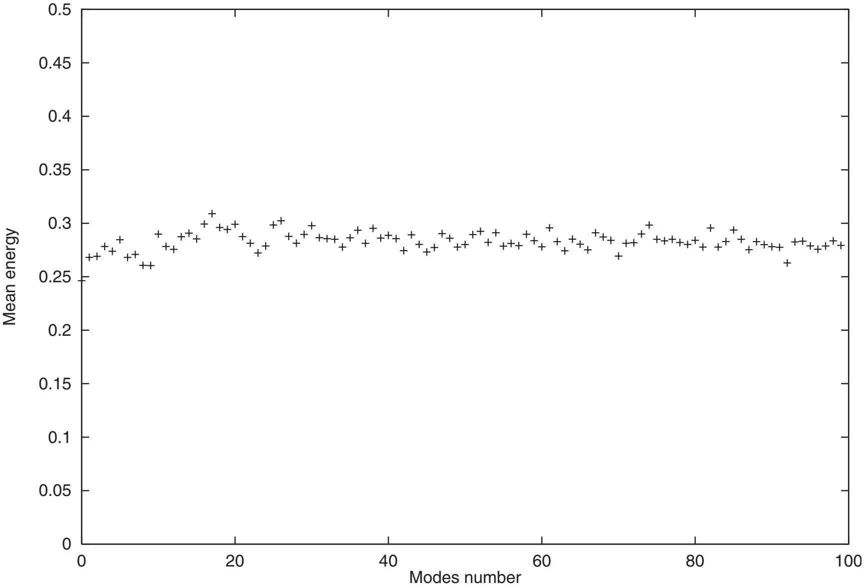

Fig. 3. Energy spectrum of the FPU system, at high temperature.

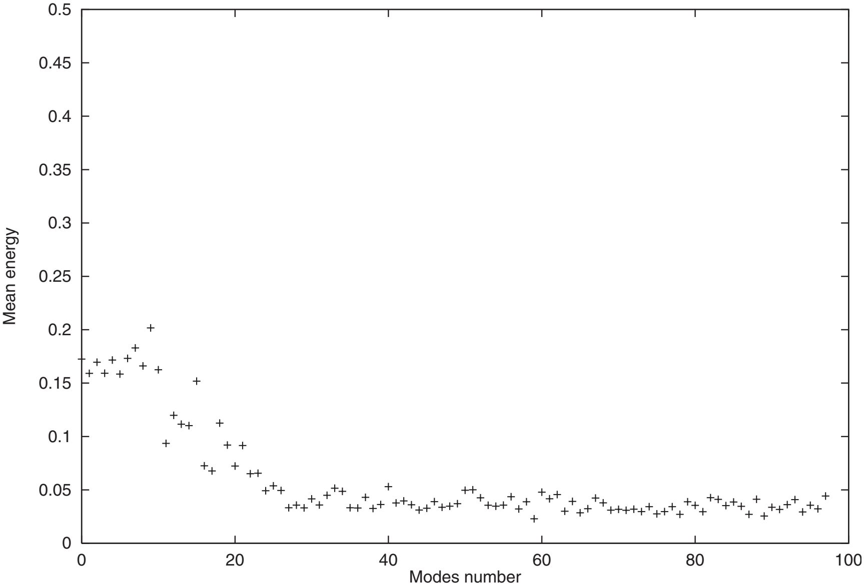

Fig. 4. Same as Fig. 3, at low temperature.

5. CONCLUSIONS

In conclusion, we hope to have shown, through our numerical study of a Fermi–Pasta–Ulam system in contact with two gases, that there are cases of metastable equilibrium for which a notion of temperature can be defined. However, at variance with the familiar case of equilibrium, such a temperature does not coincide with the "canonical" one, namely twice the mean kinetic energy per particle.

This has a certain analogy with the case of glasses. We notice however that the metaequilibrium states met in Fermi–Pasta–Ulam systems present characteristics which are somehow opposite to those of glasses. Indeed, in the latter case the lack of thermalization is ascribed to the low frequency modes and correspondingly the thermometer measures the mean energy of the high frequency modes, which are the one being in mutual equipartition.

We give now a comment concerning the relations with some recent works that also deal with the dynamics of nonlinear chains coupled to heat baths, in particular two heat baths.(9) For a review see ref. 10. We point out first of all that in all such works the main problem is very different from the present one. Indeed one looks there for the approach to an equilibrium (or stationary) state, so that the prossible existence of metaequilibrium states, which is the main object of the present work, is not even considered. A further difference concerns the interaction with the heat bath. Indeed, the models of interaction considered in all those papers are of two types. The first one amounts essentially to add to the chain a white noise, with the consequence that all normal modes of the chain are equally excited. This is qualitatively different from the present model, because we consider smooth collisions with particles (mimicking an ideal gas), with the consequence that the excitation of the different modes decays exponentially with the mode frequency; this is an essential ingredient for the establishment of a metaequilibrium state involving only the low frequency modes. A second class of works mimicks the reservoir through the so called Nosé–Hoover thermostat. The connection with our model is not clear, at least to us.

These are the differences. In any case, we have to mention that in the review article(10) it is pointed out that the mean kinetic energy should not necessarily be identified with temperature, which is indeed the main point made in the present paper.

As a final comment, we would like to mention that the possibility of having a thermodynamics for situations of metaequilibrium, typically involving the presence of adiabatic invariants, was amply discussed in the second part of a very interesting paper of Poincaré,(11) which appears to have been almost completely forgotten. In fact we became aware of such a paper only after completing the present work, through a conference of

V. Kozlov.(12) In fact, V. Kozlov was addressing only the problem dealt with in the first part of the paper of Poincaré, namely how it occurs that the fast variables of an integrable hamiltonian system approach equilibrium, notwithstanding the reversibility and the return property of the system. In the second part of his paper, Poincaré was instead considering a situation in which one has at first a quick relaxation to a "provisional equilibrium" while a "definitive equilibrium" would be attained after a much larger time, i.e., one is concerned, in his very words, with "very long times of first order" and "very long times of second order," which is a situation analogous to the one discussed in the present paper.

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