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On the problem of energy equipartition for large systems of the Fermi–Pasta–Ulam type: analytical and numerical estimates

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We report on some analytical and numerical results on the exchanges of energy in systems of the Fermi–Pasta–Ulam type, in the light of Nekhoroshev's theorem, with particular attention to the dependence of the estimates on the number n of degrees of freedom. For the ordinary FPU problem we look for a control of the single normal mode energies, and we find both the analytical and numerical estimates to agree in predicting that the energy exchanges of the single modes cannot be controlled in the thermodynamic limit. We consider then a modified FPU model, with alternating light and heavy particles, which appears as composed of two subsystems, of low (acoustic) frequency and of high (optical) frequency respectively. We try to control the exchange of the total energy of the high frequency modes up to times increasing exponentially with the frequency. In this case the numerical estimates are stronger than the available analytical ones, and give indications for nonequipartition with constants essentially independent of the number n of degrees of freedom.

1. Introduction

Since the time of Fermi, Pasta and Ulam, one is confronted with the problem of knowing whether equipartition of energy for chains of nonlinearly coupled oscillators holds in the thermodynamic limit (number of degrees of freedom tending to infinity, with finite specific energy). After the original FPU results [1] and the classical work of Izrailev and Chirikov [2], the thesis that equipartition may fail in the thermodynamic limit was first proposed by Bocchieri et al. [3]. A numerical support to such a thesis then came from various works (see for example refs. [4,5,7,8]) although the situation seems not to be completely settled; see the works [9] and [10].

For a clearer understanding of the problem, and in order to make the question more precise, it is essential to have a sound theoretical framework. We consider here the point of view of perturbation theory, where one tries to control the variation with time of some relevant quantities, in the sense for example that the modulus of the variation should be less than a constant; quantities which have controlled variations will be said to be *frozen*. The first possible framework is that of the celebrated KAM theorem, where one tries to have a control (or *freezing*) for *all* times, by looking for invariant surfaces (tori), although not for all initial data. Now, the common belief is that it should not be possible to extend such a theorem to the thermodynamic limit for systems of the FPU type, at least for a relevant set of initial data; see however [11]

and [12] for other kinds of systems. Another framework, which goes back to Boltzmann [13], Jeans [14] and Littlewood [15], is that of Nekhoroshev's theorem [16]. Here one looks for a freezing only over a *finite* but large time interval, which typically increases exponentially with the inverse of a "small parameter" ε; in such a case one can find results holding for open sets of initial data. Here too the common opinion was against the possibility of having freezing in the thermodynamic limit, due to the dependence of the estimates on the number n of degrees of freedom. Indeed the estimated stability time for generic nearly integrable Hamiltonian systems has the typical form

$$T = T_* \exp(\varepsilon_*/\varepsilon)^d , \tag{1}$$

where T_*, ε_* and d are parameters depending on n; and if one uses naively the estimates that can be found in the original formulation of Nekhoroshev one gets $d \simeq 1/n^2$, so that the exponential dependence would disappear in the thermodynamic limit.

In the present paper we give some new results on the exchanges of energy in systems of the FPU type, in the light of the Nekhoroshev theorem, looking in particular at a strict control of the dependence of the estimates on the number n of degrees of freedom. Such a study is suggested by the following remarks.

(i) Remaining in the ordinary approach, where one tries to control *separately all* the actions of the system, one might hope to have an improvement in the results by working out the estimates for a specific system, and not just using the estimates for a generic one. In particular, in the special case of a system in the neighbourhood of an equilibrium point, like the FPU problem, some improvements might be expected because the so called "geometric part" of Nekhoroshev's theorem is not needed.

(ii) Instead of trying to control separately the variation of the energies of *all* modes, as is done in the standard approach of item (i), one can look for a freezing of the total energy of a subsystem constituted by *a group* of modes. Indeed, such a weaker requirement, applied to a system of identical diatomic molecules, was shown both numerically [18] and analytically [19] to lead to estimates of Nekhoroshev type, but with the quite relevant improvement that one gets $d = 1$. This was obtained by exploiting the fact that in that case all frequencies of the considered group of modes were equal, i.e., one had exact resonance.

In section 2 we study the classical FPU model from the point of view of item (i), which is the classical one of perturbation theory. We report the analytical estimates for the parameters T_*, ε_* and d, which follow from some recent analytical work [20], where the theory is adapted to systems around an elliptic equilibrium; this leads in particular to $d \simeq 1/n$. Moreover, we show by numerical computations, for systems with n ranging from 4 to 120, that such analytical estimates are essentially optimal. The conclusion is then that there should be no hope to get positive results for the freezing of the separate energies of all the normal modes, by naively extending classical perturbation theory to the thermodynamic limit for the FPU system.

In section 3 we obtain the main positive result of the present paper, by approaching the problem from the viewpoint of item (ii), i.e., by looking for a freezing of the total energy of a subsystem constituted by a suitable group of modes. In fact, here we are confronted with the quite delicate problem that we are unable up to now to find a natural separation of the FPU system in suitable subsystems to which a Nekhoroshev-like result in the form of ref. [19] can be applied; this difficulty was also remarked in some numerical computations by Kantz [9]. However, it is well known in solid state physics that there exists a very simple variant of the FPU model in which one has a clear cut separation in two subsystems; this is the model with alternat-

ing heavy and light particles, where the frequency spectrum separates out into an "acoustical branch", with low frequencies, and an "optical branch", with high frequencies. In such a model one can then try to control the energy exchanges between the corresponding two subsystems along the lines of refs. [19] and [18], and indeed we find analytical estimates of Nekhoroshev's type, with exactly $d = 1$. For the remaining parameters we are only able to get analytically $T_* \simeq 1/n^6$ and $\varepsilon_* \simeq 1/n^8$; however, by numerical computations with n ranging from 4 to 200 we find indications that ε_* might be independent of n, while T_* should decrease less than $1/\ln n$. If this is true, then even for macroscopic systems with $n \simeq 10^{23}$ one would have no equipartition between the two subsystems for significantly large times.

2. Freezing of the harmonic actions in the FPU model

2.1. Results from classical perturbation theory

In the present section, we consider the well known FPU α model, namely a chain of $n+2$ equal particles on a straight line with nearest neighbours coupling, due to equal springs having a harmonic part and a *cubic* perturbation; as in the original work of Fermi, Pasta and Ulam, the ends of the chain are fixed. The Hamiltonian of the model is

$$H = \frac{1}{2}\sum_{j=0}^{n}[y_j^2 + (x_{j+1} - x_j)^2] + \frac{\alpha}{3}\sum_{j=0}^{n}(x_{j+1} - x_j)^3 , \tag{2}$$

where x_j is the displacement of the jth particle from its equilibrium position, and y_j the corresponding conjugate momentum. The mass of the particles and the elastic constants of the springs have been set equal to 1. Analogously, the constant α too will be set equal to 1; in fact, this simply corresponds to a suitable choice of the units of mass, length and time.

The characteristic frequencies of the linearized system are

$$\omega_l = 2\sin\tfrac{1}{2}k_l , \quad 1 \le l \le n , \tag{3}$$

where

$$k_l \equiv k_l(n) = \frac{l\pi}{n+1}$$

are the wave numbers. The canonical transformation to the normal modes q_l of the linear part and to the corresponding conjugate momenta p_l is

$$q_l = \sqrt{\frac{2}{\omega_l(n+1)}}\sum_{j=1}^{n} x_j \sin\left(\frac{jl\pi}{n+1}\right) ,$$

$$p_l = \sqrt{\frac{2\omega_l}{n+1}}\sum_{j=1}^{n} y_j \sin\left(\frac{jl\pi}{n+1}\right) . \tag{4}$$

This brings the Hamiltonian into the form

$$H = H_2(p, q) + \alpha H_3(q) , \tag{5}$$

with

$$H_2 = \frac{1}{2}\sum_{l=1}^{n}\omega_l(p_l^2 + q_l^2) , \tag{6}$$

which corresponds to a system of harmonic oscillators (normal modes), with a coupling due to a suitable perturbation H_3, the explicit expression of which is however not relevant here.

The classical perturbative approach consists in trying to build up a set of n independent first integrals $\Phi^{(l)}(q, p)$ which are perturbations of the harmonic actions

$$I_l = \tfrac{1}{2}(p_l^2 + q_l^2)$$

of the system, namely

$$\Phi^{(l)} = I_l + \Phi_3^{(l)} + \Phi_4^{(l)} + \cdots , \quad l = 1, \ldots, n . \tag{7}$$

where $\Phi_s^{(l)}$ is a homogeneous polynomial of degree s. The formal equation for each first integral is $\{H_2 + H_3, \Phi^{(l)}\}$, where $\{\cdot, \cdot\}$ is the Poisson bracket. This leads to a formal expression for each first integral, which is determined by recursively solving the equations

$$\{H_2, \Phi_s^{(l)}\} = -\{H_3, \Phi_{s-1}^{(l)}\} \tag{8}$$

(here $\Phi_2^{(l)} = I_l$).

The formal consistency of the construction can be proven at all orders if the harmonic frequencies are nonresonant, i.e. if one has $k \cdot \omega \neq 0$ for $k \in \mathbb{Z}^n/\{0\}$; for the proof see refs. [21] and [20], which refer to the common case, as is ours, of a Hamiltonian even in the momenta. We are well aware of the problem that for certain values of n one actually has resonance in the present model; however we found that this is essentially irrelevant for our purposes.

Now, the power expansions (7) of the first integrals are known to be generally not convergent. On the other hand, in a suitable domain one can build up a set of n quasi integrals of motion (*adiabatic invariants*), which are functions $\Phi^{(l)}$ of the form (7), where however the sum is extended up to a suitable optimal order r_{opt}; for the time derivative of such quasi integrals one finds an exponential estimate. More precisely, let us consider domains of the form

$$\mathcal{D}_\rho = \{(p, q) \in \mathbb{R}^{2n} : |p_l| \leq \rho, |q_l| \leq \rho, 1 \leq l \leq n\}, \tag{9}$$

namely polydisks of radius ρ centered at the origin. Then there exists ρ_0 such that, given ρ in the interval

$$0 < \rho < \rho_0, \tag{10}$$

for any $(p, q) \in \mathcal{D}_\rho$ one can choose r_{opt} as a function of ρ, and one gets the bound

$$|\dot{\Phi}| \equiv \max_l |\dot{\Phi}^{(l)}| < b(\rho) \equiv a \exp(-\mu/\rho^c), \tag{11}$$

with suitable constants a, μ and c. This is nothing but the exponential estimate (1) of the stability time, with corresponding constants T_*, ε_* and d.

Notice that, in the spirit of perturbation theory, ρ_0 is to be considered as the analogue of a stochasticity threshold. Indeed, for $\rho > \rho_0$ already the first order approximation of the adiabatic invariant turns out to be worse than the harmonic action itself, in the sense that no bound on the variation of the actions can be given. In this sense, this is the lower estimate of a stochasticity threshold, which is afforded by perturbation theory.

As to the dependence of the constants on the number n of degrees of freedom, in which we are particularly interested, by a simple application of the formalae given in ref. [20] one gets, for large n,

$$c \sim \frac{1}{n}, \quad \mu \sim n, \quad \ln a \sim n, \tag{12}$$

and $\rho_0 \sim \rho_*/3^n$ with a suitable ρ_* which, in the FPU α model, behaves as $n^{-5/2}$; thus one has

$$\rho_0 \sim (3^n n^{5/2})^{-1}. \tag{13}$$

In order to have informations on the thermodynamic limit $n \to \infty$ at fixed specific energy $E/n = \text{const.}$, it is essential to estimate how the parameter ρ controlling the domain depends on the energy E. To this end, recall that ρ is defined as the radius of a polydisk in $\mathbb{R}^{2n}$ where the orbit is required to be confined for all times for which the estimates should be valid; on the other hand $\rho^2/2$ is the maximum value of the action that can be reached by a single oscillator. So, the most natural choice is

$$\rho = \sqrt{2E/\omega_1}. \tag{14}$$

Thus, the condition $\rho < \rho_0$ required to apply the perturbation theory implies $0 < E < E_0$, where, due to (13) and to $\omega_1 \sim 1/n$ (see (3)), one has

$$E_0 \sim (9^n n^6)^{-1}. \tag{15}$$

In conclusion, we have the result that the exponential stability time is guaranteed analytically within a domain of energy which is estimated to shrink to zero in the thermodynamic limit.

The problem is now to understand whether the analytical estimates are optimal. This is a hard mathematical problem, to which apparently there is no answer at the moment. Thus we come to a numerical investigation, with the aim of getting rough indications, which should just be considered as possible suggestions for future mathematical work.

So, we try to estimate numerically the quantity $b(\rho)$ which bounds $|\dot{\Phi}|$ from above. Here, one has to tackle the severe problem that the explicit expansion of the adiabatic invariants $\Phi^{(l)}$ is actually impractical for large n, so that in practice one can handle only the harmonic actions I_l, which are just the first order approximations to them.

So the problem is to introduce suitable quantities, defined in terms of the harmonic actions I_l, through which one can test the analytical estimates. By the way, from a point of view of principle one could also reverse the situation, because one might maintain that the quantities of physical relevance should just be the harmonic actions (or the corresponding harmonic energies) themselves, and so it would be sound to find analytical bounds for the variations of the harmonic actions. In any case, the relation between the bound on the harmonic actions I_l and the bound on the adiabatic invariants $\Phi^{(l)}$ comes about from the relation

$$\begin{aligned} &|I_l(t) - I_l(0)| \\ &\quad \le |I_l(t) - \Phi^{(l)}(t)| + |\Phi^{(l)}(t) - \Phi^{(l)}(0)| \\ &\quad + |\Phi^{(l)}(0) - I_l(0)| \,. \end{aligned} \tag{16}$$

This naturally leads to consider two separate contributions to the time variation of the harmonic actions, namely:

(i) the deformation $|I_l - \Phi^{(l)}|$, which is due to the fact that the harmonic actions are just an approximation of the adiabatic invariants $\Phi^{(l)}$; such a contribution would occur even if the power expansion for the first integrals were convergent;

(ii) the noise (or *diffusion*) $|\Phi^{(l)}(t) - \Phi^{(l)}(0)|$, which is due to the fact that the time derivative $\dot{\Phi}^{(l)}$ is not zero, just because $\Phi^{(l)}$ is a truncated and not a true integral.

So one has to take into account both contributions. An analytic estimate for the deformation can be found in ref. [20]: precisely, at any point of the domain $\mathcal{D}_\rho$ defined above one can prove

$$\max_l |I_l - \Phi^{(l)}| < \delta(\rho) \equiv \delta_* \rho^3 \,, \tag{17}$$

with a suitable constant δ_*. The estimate for the noise is instead given by (11) and (12).

In the next section we will introduce two quantities $\tilde{\delta}(\rho)$ and $\tilde{b}(\rho)$, which are defined in terms of just the harmonic actions, and that we consider somehow as the analogues of the quantities $\delta(\rho)$ and $b(\rho)$.

2.2. Numerical results

We integrated numerically the equations of motion with the number n of particles ranging from 4 to 120, for t up to $2^{15} T_1$, where

$$T_1 = 2\pi/\omega_1 \tag{18}$$

is the period of the slowest mode (which, by the way, depends on n); in particular, we looked at the instantaneous values of the harmonic actions $I_l(t)$, $l = 1, \ldots, n$. As in the papers [3–5], we used the standard central point method (namely the simplest symplectic integrator available: see also [6]), working on a VAX computer; usually, the computations were in single precision, and the total energy was conserved within 3%; some runs were also performed with double precision and smaller integration steps in order to check the results, and we found no significant differences.

The main goal of our investigation was to check whether or not the qualitative behaviour (especially the dependence on n) of the analytic estimates recalled above for the variation of the actions were, in some sense, optimal. In particular, we had to distinguish between the contribution due to deformation and the one due to noise. Now, in the limit of small energies, observing that ρ^2 is essentially the maximal possible value of each harmonic action of the system, from the formulae (16), (11) and (12) one clearly sees that, for short times, the effect of the deformation should be prevailing with respect to that of noise. Indeed, the effect of noise is exponentially small with $1/\rho$; moreover, the deformation manifests itself in a few harmonic periods, since it essentially corresponds to a motion on a deformed torus. By the way, this is one of the main reasons which makes it difficult to reveal the noise itself, if one is able to measure just the harmonic actions.

The effect of the deformation is well exhibited in the classical figures of Fermi, Pasta and Ulam; see fig. 1, where the time evolution of some of the harmonic energies $\omega_l I_l$ for $n = 6$ are reported: the essentially periodic oscillations, with period $2\pi/\omega_1$, are clearly due to the fact that the orbit is very close to a deformed torus, which in turn is close to a torus of the unperturbed system with Hamiltonian $H_2(p, q)$.

The long time effect due to noise, which superimposes itself to the rapid deformation, is well illustrated in fig. 2, which gives the maximum and the minimum of the harmonic action I_4 vs. time; the data are $n = 6$ and initial equipartition of energy among the modes, with specific energy 10^{-5} (top) and 10^{-3} (bottom). This figure confirms very well that one has two distinct phenomena occurring at two well separate time scales. The problem is now to find a suitable

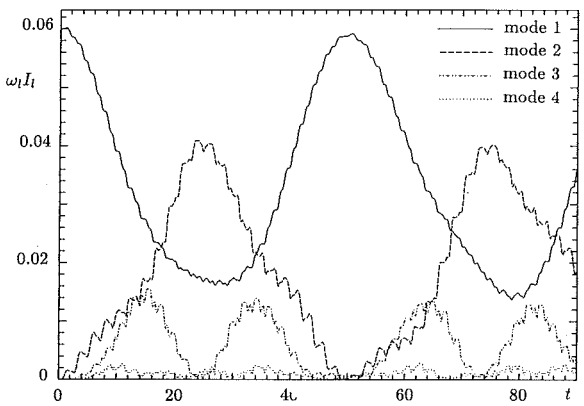

Fig. 1. Time evolution of the harmonic energies of the first four modes in a chain of 6 particles. Initial data: total energy $E_0 = 0.06$, with just the lowest frequency mode excited; time unit: the period of the fastest oscillator. The figure exhibits the effect of the deformation, which causes the quasiperiodic behaviour of the harmonic energies.

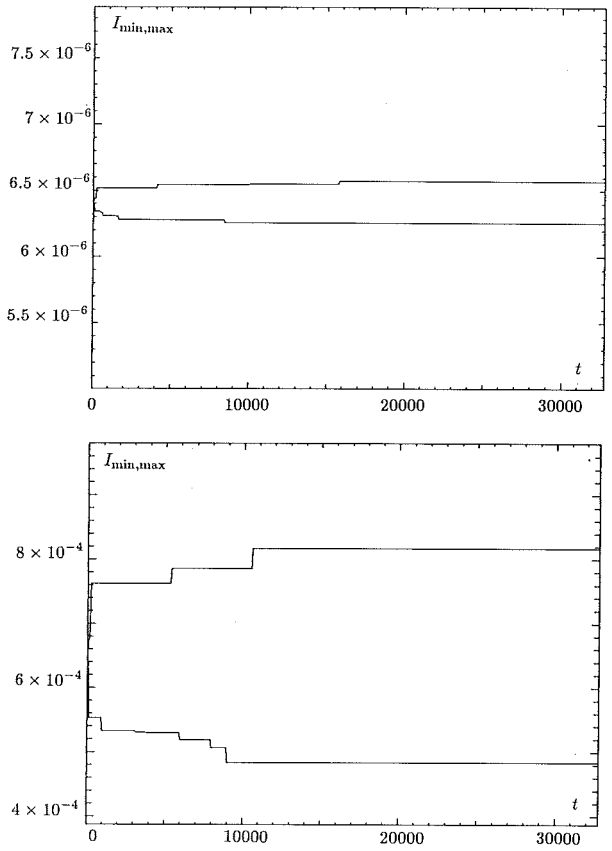

Fig. 2. Maximum and minimum value of the harmonic action I_4 of the fourth mode vs. time. The figure shows that there are two separate phenomena occurring on different time scales: the deformation causes the quite fast spreading of the curves; the noise causes the slow change of the values over a large time scale. Initial data: equipartition of energy, with specific energy 10^{-5} (top) and 10^{-3} (bottom).

method to exhibit the presence of such two time scales in a more quantitative way.

Let us now come to the details, by first working at a fixed n. The analytic estimates we are checking are the ones given by (17) and (11), which bound the maximum of the deformation $|I_l - \Phi^{(l)}|$ and the maximum of the diffusion speed $|\dot{\Phi}^{(l)}|$ as functions of ρ. So we have to explain how we numerically estimate the quantities $\delta = \delta(\rho)$ and $b = b(\rho)$, which bound the deformation and the diffusion speed, by making use of just the harmonic actions; we assume the relation between ρ and the total energy E given by (14).

Let us consider the numerical estimate of $\delta(\rho)$. We notice that, as shown by formula (16), if the adiabatic invariant were exactly constant, then $|I(t) - I(0)|$ would be bounded by twice the deformation. So, due to the fact that the adiabatic invariant is in fact practically constant for short times, we can guess that a good estimate for the deformation is just one half the maximal fluctuation of the harmonic action up to not too long times; such a guess is supported by fig. 2, which clearly shows that the main effect of the deformation manifests itself in quite short times. So, we evaluate the deformation in the following way. Consider the two straight lines fitting the maximal and the minimal values of $I_l(t)$ for not too short times, and get their intersections with the ordinate axis; then we introduce the quantity $\tilde{\delta}(\rho)$, defined as the maximum over l of half the distance between such intersections, and consider this as a *bona fide* quantity that should numerically estimate $\delta(\rho)$. The fitting was actually performed after discarding the values $I_l(t)$ for $t < 100\ T_1$, with T_1 as in (18), as is suggested by fig. 2.

Let us finally come to the numerical estimate for the quantity $b(\rho)$, which measures the noise. By the same reasons as above, in virtue of relation (16), the quantity $b(\rho)$ might be estimated numerically by the absolute value of the slope of the straight lines just described. However, such an estimate turns out to be too rough, because one should be able to wash out the contributions to such lines due to the low-frequency components of the deformation. After some trials, we found that a good *bona fide* estimate $\tilde{b}$ for b is given by the quantity

$$\tilde{b} = \max_l \sup_t \left| \frac{I_l(t + \Delta t) - I_l(t)}{\Delta t} \right| ,$$

for a suitable choice of Δt. We checked that the results do not significantly change for Δt ranging from $10\ T_1$ to $50\ T_1$.

The method just described to estimate b by $\tilde{b}$ might be justified by a clever understanding of the origin of the distinction between deformation and noise in perturbation theory. To this end, one should recall that in the Nekhoroshev-like theory one exploits the asymptotic character of the series expansions of the first integrals, which behave practically as convergent series for low orders; in fact, the adiabatic invariants are just those series truncated at a suitable order, where they "start to diverge". If the adiabatic invariants were exactly constant, then the harmonic actions $I_l(t)$ would be quasi periodic functions of time with frequencies $k \cdot \omega$, where $|k| \equiv |k_1| + \cdots + |k_n|$ is less than the truncation order. This is actually the deformation. Notice that the amplitudes of such quasi periodic components decrease rapidly with $|k|$, due to the practically convergent character of the series at low orders. This is no more true for the components with large values of $|k|$, which cannot be controlled by perturbative methods, and are in fact collected in the noise. Thus, one can try to wash out the deformation by averaging $\dot{I}_l(t)$ over a suitable period Δt, which should be a not too large multiple of T_1. This is clearly the basis of our method.

Let us now come to the numerical results. In fig. 3 we report the computed values of $\tilde{\delta}$, for ρ in the range 10^{-3} to 1 and for $n = 6$, in Log–Log scale (here, Log denotes decimal logarithm). The data are well fitted by a straight line with slope ~ 2.7, which is quite well in agreement with

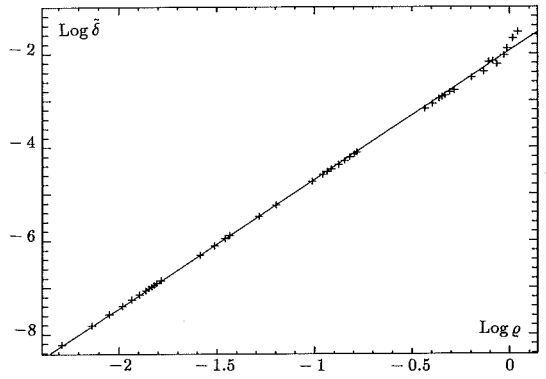

Fig. 3. Numerical estimate of the deformation $\tilde{\delta}(\rho)$ vs. ρ. The data are in good agreement with the theoretically expected behaviour, given by (17). Initial data: $n = 6$, with equipartition of energy among all modes. The value of ρ is related to the total energy by (14)..

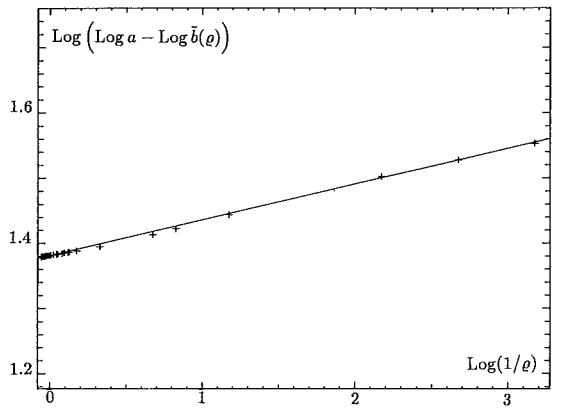

Fig. 5. Same as fig. 4, in logarithmic scale, in order to bring into evidence the exponential behaviour, according to the theoretical estimate (11). Initial data as in fig. 3.

the estimated value of 3. The data for the function $\tilde{b}(\rho)$, are reported in fig. 4, with ρ in the same range as above, and still $n = 6$. In order to exhibit in a figure the exponential dependence on $1/\rho$, we first estimate from the numerical data, by best fit with the formula (11), the values of the constants a, μ and c, and then report in fig. 5 a plot of Log a − Log $\tilde{b}(\rho)$ vs. ρ in Log–Log scale. As one sees, the points are well aligned along a straight line, in agreement with the theoretical expectation.

We come now to a discussion of the dependence of the values of the constants a, μ and c on the number of degrees of freedom n. We refer to figs. 6, 7, and 8, where log a, μ and c respectively are plotted vs. n, for n in the range 4 to 120. One sees that, at least for n larger than 40, the data seem to be reasonably consistent with the theoretical estimates given by (12).

Thus, our computations show that the analytic estimates for the freezing of the separate energies of all oscillators, given by perturbation theory, are close to being optimal as the dependence of a, μ and c on the number n of degrees of freedom. In particular, this might be considered to support also the theoretical estimate (15) for the energy threshold below which perturba-

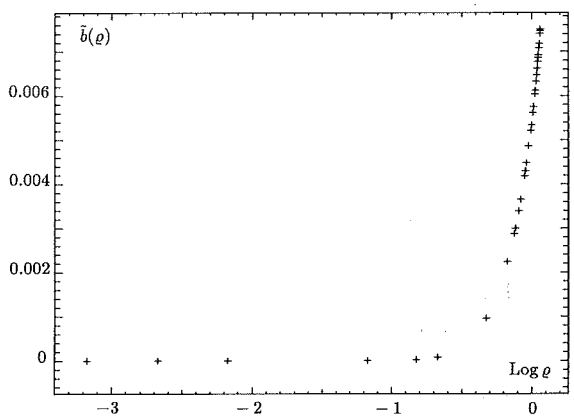

Fig. 4. Numerical estimate of the effect of the noise, to be compared with the theoretical estimate (11). Initial data as in fig. 3.

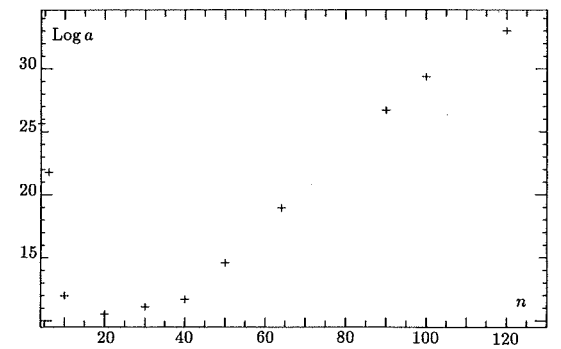

Fig. 6. Numerical estimate of the quantity a in (11) vs. n, to be compared with the theoretical estimate (12). The theoretical estimate seems to be confirmed for large n.

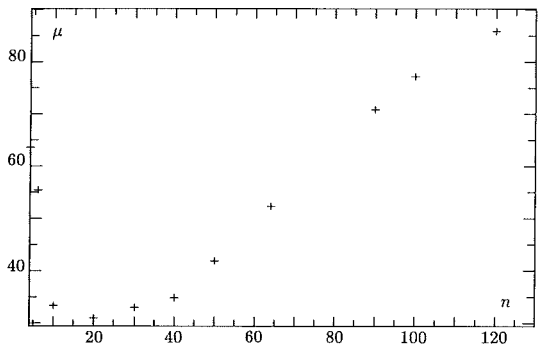

Fig. 7. Numerical estimate of the quantity μ in (11) vs. n, to be compared with the theoretical estimate (12). The theoretical estimate seems to be confirmed for large n.

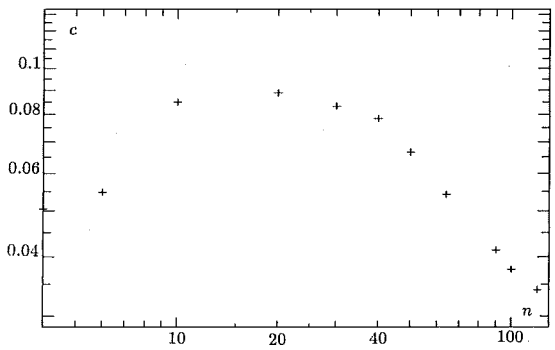

Fig. 8. Numerical estimate of the quantity c in (11) vs. n, to be compared with the theoretical estimate (12). Although the expected behaviour $c \sim 1/n$ cannot be considered as fully confirmed, it seems nevertheless reasonable to conclude that c decreases to zero with increasing n.

tion theory can be applied; this means that one should have freezing of all the harmonic actions only in an energy interval which shrinks to zero in the thermodynamic limit.

In this sense one might say that the numerical computations discussed above appear to lend support to the thesis that, even if one takes the point of view of Nekhoroshev instead of KAM, there is no freezing of the separate harmonic energies of the harmonic oscillators in the thermodynamic limit $n \to \infty$. However, there remains the possibility of a freezing of the total energy of suitable packets (or groups) of oscillators, as we are going to discuss in section 3.

3. Freezing of the subsystem of high frequency modes in the modified FPU model

3.1. Description of the model

We consider here the modified FPU β-model which, for an even number n of particles, is described by the Hamiltonian

$$H = \frac{1}{2}\sum_{j=0}^{n}\left(\frac{y_j^2}{m_j} + (x_{j+1} - x_j)^2\right) + \frac{\beta}{4}\sum_{j=0}^{n}(x_{j+1} - x_j)^4 , \tag{19}$$

with $m_j = 1$ for j odd and $m_j = m < 1$ for j even; we still consider fixed ends. With respect to the Hamiltonian considered in section 2, the interaction potential is now a quartic one (we actually worked with $\beta = 1$). This is however irrelevant, and the major difference consists instead in the choice of the alternating masses, because this is very well known to lead to a frequency spectrum with disjoint branches, that are usually called the acoustic one and the optical one. Indeed, the characteristic frequencies of the linearized system are well known to be given by

$$\omega_l^2 = \frac{1 + m \pm \sqrt{1 + m^2 + 2m\cos 2k_l}}{m} , \quad 1 \le l \le n/2 , \tag{20}$$

where

$$k_l = \frac{l\pi}{(n+1)}$$

still are the wave numbers. In fig. 9 we plot the dispersion law ω vs. k for different values of the "small mass" m, namely $m = 1$, 0.7, 0.3 and 0.1. For $m = 1$ one has the standard dispersion relation of the FPU model, while for $m < 1$ one has two different branches: for $0 < k < \pi/4$ one has the so called acoustic branch which is only slightly modified with respect to the standard one, while for $\pi/4 < k < \pi/2$ one has the optical

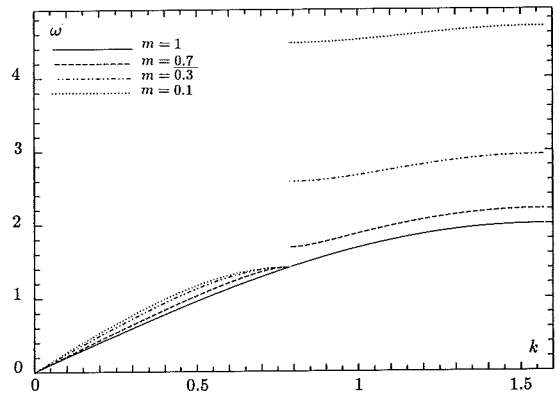

Fig. 9. Dispersion law ω vs. k for the modified FPU model, for different values of the mass parameter. The figure clearly exhibits the separation of the acoustic and the optical branches.

branch, which separates out from the standard one, lying above it. Notice that, with decreasing m, the gap between the two branches increases, and moreover the optical branch becomes flatter and flatter; in other words one obtains two well separate subsystems of harmonic oscillators, the optical subsystem being constituted of oscillators of essentially the same frequency. Precisely, defining the gap $\Delta\omega$ as the difference between the minimal optical frequency and the maximal acoustic frequency, one gets

$$\Delta\omega = \sqrt{2}\left(\sqrt{\frac{1}{m}} - 1\right);$$

analogously, for the width $\delta\omega$ of the optical branch, defined in the obvious way as the difference between the maximal and the minimal optical frequencies, one gets

$$\delta\omega = \sqrt{\frac{2}{m}}\,(\sqrt{1+m} - 1)\,,$$

and so

$$\delta\omega \sim \sqrt{\frac{m}{2}} \quad \text{for } m \ll 1\,.$$

To determine the canonical transformation to the normal modes, we order the frequencies as $(\omega_1^-, \ldots, \omega_n^-, \omega_1^+, \ldots, \omega_n^+)$, where the + and − refer to the choice of the sign in (20); then we introduce the coordinates q_l and the conjugate momenta p_l of the normal modes via the canonical transformation

$$x = Rq\,, \quad y = (R^{-1})^{\mathrm{T}} p\,, \tag{21}$$

where R is the matrix with elements

$$R_{jl} = \frac{2}{\sqrt{n+1}} \sqrt{\frac{2}{|2 - m_j \omega_l^2|}}\,|\cos k_l| \times \frac{\sin(j \cdot k_l)}{(1 + m^2 + 2m\cos 2k_l)^{1/4}}\,,$$

and the upper index T denotes transposition.

3.2. *Analytic results from perturbation theory*

In the spirit of the works [18] and [19], instead of trying to control separately the energy of each oscillator, we try to control the energy exchange between the subsystem of the acoustic modes and the subsystem of the optical modes; actually, one can work out analytically such a program by slightly modifying the two subsystems, as will now be explained. Indeed, in the analytical paper quoted above one considered an Hamiltonian of the form

$$H = h_\omega(\pi, \xi) + \hat{h}(p, x) + f(p, x, \pi, \xi)\,, \tag{22}$$

where $h_\omega(\pi, \xi)$ is the Hamiltonian of a certain number of harmonic oscillators, all of the same frequency ω, $\hat{h}(p, x)$ is the Hamiltonian of another arbitrary system, while $f(p, x, \pi, \xi)$ is a coupling term, which is required however to be small with ξ; one is interested in the exchange of energy between h_ω and $\hat{h}$ for large ω. In our case h_ω should correspond to the system of oscillators of the optical branch and $\hat{h}$ to the system of oscillators of the acoustic branch, so that the variables π, ξ and p, x describe the oscillators of the optical and of the acoustic branches respec-

tively. This, however, is insufficient because on the one hand the optical frequencies are not all equal, and on the other hand the quartic part of the Hamiltonian turns out not to vanish with ξ. So, in order to conform to the above splitting, we further decompose the harmonic energy of the optical branch into a system of harmonic oscillators of the same frequency ω (equal to an average of the frequencies of the optical branch), which is identified with h_ω, and into a corresponding remainder, which is included in the coupling f. Moreover, the part of the quartic term which is independent of the variables ξ is also included in $\hat{h}$. Thus, we decompose our original Hamiltonian H as in (22), with

$$h_\omega(\pi, \xi) = \frac{1}{2}\sum_{l=1}^{n/2}(\pi_l^2 + \omega^2\xi_l^2)\,,$$

$$\hat{h}(p, x) = \frac{1}{2}\sum_{l=1}^{n/2}(p_l^2 + \omega_l^2 x_l^2) + H_4^0(x)\,,$$

$$f(x, \xi) = \frac{1}{2}\sum_{l=1}^{n/2}(\varepsilon_l^2 + 2\varepsilon_l\omega)\xi_l^2 + H_4'(x, \xi)\,; \quad (23)$$

here we have introduced the quantities

$$\omega^2 = \tfrac{1}{2}[(\omega_{\max}^+)^2 + (\omega_{\min}^+)^2]\,,$$

$$\varepsilon_l = \omega_l - \omega\,,$$

where $\omega_{\max}^+$ and $\omega_{\min}^+$ are the maximal and the minimal optical frequencies respectively; moreover H_4^0 is the part of the quartic term in the Hamiltonian which does not depend on ξ, while H_4' is the remaining part of it.

For an Hamiltonian of the form (22), the analytic results concerning the exchange of energy between h_ω and $\hat{h}$ are obtained by still constructing a quasi integral of motion (or adiabatic invariant) Φ, which is a perturbation of h_ω; a convenient dimensionless parameter characterizing the optical branch is

$$\lambda = \frac{\omega}{\omega_{\max}^-}\,, \quad (24)$$

where $\omega_{\max}^-$ is the maximal acoustic frequency. Using the results of ref. [19], one finds that one can apply perturbation theory (i.e. one has freezing) for λ in the interval

$$\lambda > CE\,, \quad (25)$$

where C is a constant depending on n, and E is the total energy; with this condition, the time derivative of Φ is bounded by

$$\lambda|\dot{\Phi}| < A\,\mathrm{e}^{-B\lambda}\,, \quad B = \frac{\mathrm{e}}{CE} \quad (26)$$

with a suitable constant A depending on n. In particular, notice that the analogue of the constant c that appeared in section 2, and that would appear here as an exponent to λ in the exponential, has now become exactly equal to 1. The quantities A and C depend on the perturbation f and on the domain in which the system is considered. Simple considerations based on ref. [19] lead to the analytical estimates

$$A \sim n^6\,, \quad C \sim n^8\,.$$

So, for a definite model, in which λ has a fixed value, one deduces that the stability estimate of exponential type would hold in an interval of specific energy which is estimated to shrink to zero in the thermodynamic limit. In this sense one could say that the theoretical estimates do not ensure freezing in the thermodynamic limit in the Nekhoroshev sense, even by considering exchanges of energy between suitable groups of modes. Conversely, if one fixes the specific energy and considers as variable λ, one has that the analytical estimates ensure an exponential bound of the type (26) only on an interval $[\lambda_*, +\infty)$, with λ_* going to infinity with n.

However, at variance with the previous case in which one was looking for the separate freezing of all modes, it turns out that the numerical computations now suggest that the theoretical estimates should be far from optimal, and one might also have freezing in the thermodynamic limit, as we now show.

3.3. Numerical results

We start by illustrating the fact that the acoustic and the optical modes form two subsystems which in general tend to separate equilibria. This is shown in fig. 10, where the time average energies of the single modes are reported versus time; initial data were: total energy on the lowest frequency mode, and $n = 8$. Let us recall that, for a system of harmonic oscillators of the same frequency (or in exact resonance), one knows that there is a significant exchange of energy among the single oscillators in a time of the order ε^{-1}, if ε is the small parameter characterizing the perturbation. For a beautiful illustration in the case of two dimensional FPU-like problem, see ref. [17]. Now, the oscillators of the optical branch are almost completely resonant, so that they very rapidly go to equipartition; the time needed is instead quite longer for the oscillators of the acoustic branch, because they have a quite wide frequency spectrum. So, it is clear that it would not be convenient to look for the separate conservation of the energy of each normal mode, while the interesting quantity is the energy exchange between the two subsystems. Thus, we should estimate the time derivative of the adiabatic invariant Φ, which is a perturbation of h_ω.

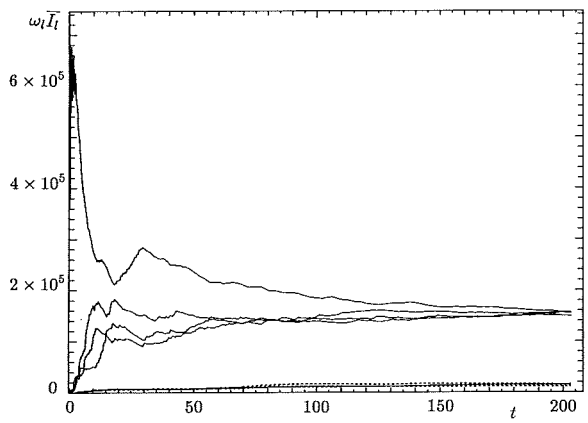

Fig. 10. Time averages of the harmonic energies of the single modes. The figure clearly exhibits the splitting of the system into the separated subsystems of the acoustic and the optical modes. Initial data: $n = 8$, with the total energy initially on the lowest frequency mode.

Due to the fact that we can actually measure, by numerical simulation, the fluctuations of just the harmonic part h_ω of Φ, and not of the adiabatic invariant Φ itself, here too we should have to isolate the separate contributions of deformation and noise; in this connection one might repeat here considerations analogous to those of part A. In fact, we proceeded in a slightly different way, aiming at checking directly the estimate (26) of $|\dot{\Phi}|$. So we computed the quantity $\dot{E}^+$ defined by

$$\dot{E}^+ = \sup_t \langle |\dot{h}_\omega(t)| \rangle \ ;$$

here the average $\langle \cdots \rangle$ is taken over several orbits corresponding to different random initial data at the same total energy, while the sup is taken over the time for which the orbits were computed. In our case the number of different orbits was 64, and each orbit was integrated for a time equal to $\frac{1}{16}$ the time of the previous case discussed in section 2. The reason why $\dot{E}^+$ should be a good estimate for the maximum of $|\dot{\Phi}|$ is simply that we need to wash out, as in the previous case, the quasiperiodic contribution due to the deformation. Here, we simply replace a time average with an average over different orbits, which turns out to be an even more convenient numerical procedure.

In order to estimate the constants A and B entering the exponential bound (26), we perform a series of numerical computations for different values of λ by fixing the specific energy $E/n = 10^6$, with n ranging from 6 to 200. In fig. 11 we report, in semilogarithmic scale, $\lambda \dot{E}^+$ vs. λ; the initial data were $n = 10$ (and so total energy $E = 10^7$), zero energy on the optical modes and equipartition of energy among the acoustic modes. As one sees, for $\lambda > 70$ the numerical results are quite well fitted by a straight line; this is in good agreement with the theoretical estimate $c = 1$, recalled above. The slope of the straight line and its intercept at the origin clearly

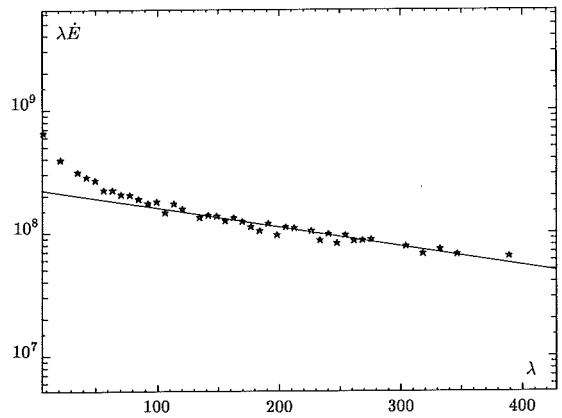

Fig. 11. Numerical estimate of $\lambda \dot{E}^+$ vs. λ, to be compared with the theoretical estimate (26). The data are in good agreement with the purely exponential estimate. Initial data: $n = 8$, and total energy $E = 10^7$, with zero energy on the optical modes and the equipartition of energy among the acoustic modes.

provide estimates for the parameters B and A, which could depend on n. Such a dependence on n is illustrated in fig. 12, where the same quantity $\dot{E}^+$ as a function of λ is reported for six different values of n, ranging from 6 to 200. Clearly, the slope is essentially the same for all cases, which suggests that B might be independent of n. In-

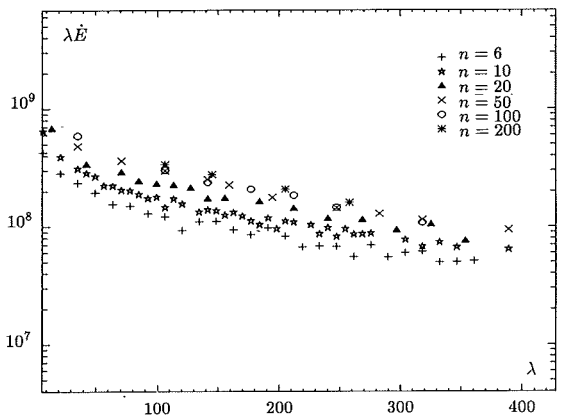

Fig. 12. Same as fig. 11, for different values of n, to be compared with the theoretical estimate (26). The data corresponding to different values of n are quite well aligned on straight lines, in agreement with the purely exponential estimate. The slope of the straight lines appears to be independent of n, which suggests $B = 1$; the intercepts of the straight lines at the origin exhibit instead a small dependence on n, which suggests a small dependence of A on n.

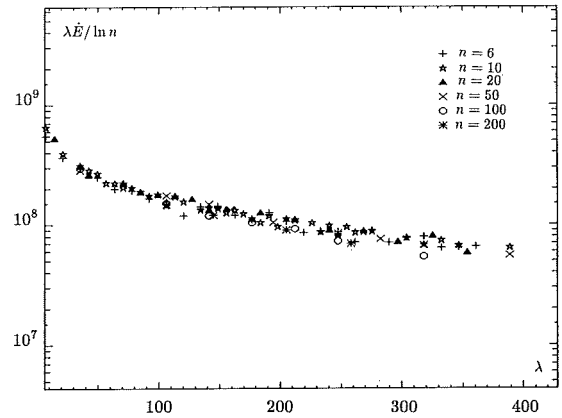

Fig. 13. Same as fig. 12, with $\lambda \dot{E}$ replaced by $\lambda \dot{E}/\ln n$, in order to check the ansatz $A \sim \ln n$. The figure shows that the increase of A with n should be less that $\ln n$.

stead, the intercept increases with n, although not so fast as in the analytical estimate. In order to have a rough estimate of the dependence of A on n, we try the *ansatz* $A \sim \mathrm{Log}\, n$; so, in fig. 13, we redraw the previous data by plotting $\lambda \dot{E}^+ / \mathrm{Log}\, n$ vs. λ. One clearly sees that there is now a change, because the intercept decreases with n. This indicates that A should in fact increase with n less than a logarithm. If this were the case, then even with a macroscopic number such as $n \simeq 10^{23}$ one would have a substantial freezing of the energy of the subsystem of the optical modes, up to macroscopic times.

4. Conclusions

In conclusion, we believe we have given strong evidence in favour of the thesis that, for macroscopic systems, nonequipartition of energy might hold for the modified Fermi–Pasta–Ulam model, characterized by alternating heavy and light particles, with the corresponding subdivision of the frequency spectrum into an acoustical branch and an optical branch. More precisely, for what concerns the exponential bound (26) on the exchange of energy between the two corresponding subsystems of virtual harmonic oscillators, the

situation is the following one. First of all, the exponent to which the frequency is raised turns out both analytically and numerically to be exactly equal to one (confirming a similar previous result [18] on a model for diatomic molecules). Then, the problem is the dependence of the two other parameters, which we have called A and B, on the number n of degrees of freedom. For them, the numerical computations seem to indicate bounds stronger than the available analytical ones, inasmuch as B might be independent of n while A should increase less than Log n.

If this were true, one might conclude that nonequipartition of energy in the above sense (namely for finite long times, in the Nekhoroshev like way, and for the energy of subsystems rather than separately for the energy of each oscillator, as first stressed in refs. [18] and [19]) should hold also for some macroscopic systems of physical interest, such as the modified Fermi–Pasta–Ulam model. So, there remains the problem to study whether it is possible to optimize the analytical estimates; this is a hard open problem.

Regarding instead the ordinary FPU problem, we have shown that the numerical estimates support the analytical prediction that the separate freezing of the harmonic energies of the oscillators cannot be extended to the thermodynamic limit. However, this clearly does not necessarily imply equipartition, because one could have freezing for suitable packets of modes with different characteristic frequencies; up to now, we were unable to find a natural decomposition into suitable subsystems. This is indeed also the problem raised in [9], which is still open.

Another comment is in order. Since the works of Izrailev and Chirikov and of Ford on the one hand, and the works of the Italian group on the other hand, one was confronted with two different theses, namely that one should have or have not equipartition in the thermodynamic limit for dynamical models of interest for statistical mechanics. Now it seems to be clear that the answer strongly depends on which particular question one asks: whether one looks for freezing in KAM sense (for all times) or in Nekhoroshev sense (for long, somehow qualitatively long, times); whether one looks for the separate freezing of all actions or for the freezing of the energy of some subsystems. In consideration of this, it is possible that theses that appeared to be mutually exclusive twenty years ago might now appear to be compatible.

If this is the case, then one obviously remains with the problem of deciding which is the correct question to be posed from the physical viewpoint. The present authors, along the lines of the works [22] and [23], clearly share the viewpoint of Boltzmann and Jeans (see [13] and [14]), according to which the freezing for qualitatively long times and for relevant subsystems should be of physical interest. But this point too should be further discussed.

We consider the present preliminary results only as indicative, and hope that in the future it will be possible to provide strict analytical estimates proving (or disproving) rigorously our thesis. In fact, the comparison made in section 2 between analytical and numerical estimates for the freezing of the separate energies of all oscillators, where a good agreement was obtained, shows that accurate analytical estimates in perturbation theory can be essentially optimal, so that the present (not too large) discrepancy of section 3 between analytical and numerical estimates might possibly be eliminated. As is well known to people working in quantitative perturbation theory, in the work of obtaining explicit estimates one has to deal, within a rather well understood general framework, with several technically delicate points where different nonequivalent choices can be made, leading to different quantitative results; for example, the space where the problem is imbedded, and the choice of suitable norms. This is a hard mathematical work to be done in the future. In the present paper we just are content with having indicated that suitable quantities are good candidates for adiabatic invariants in the thermodynamic limit.

References

[1] E. Fermi, J. Pasta and S. Ulam, Los Alamos Report No. LA-1940 (1955), later published in E. Fermi: Collected Papers (Chicago, 1965), and Lect. Appl. Math. 15, 143 (1974).

[2] F.M. Izrailev and B.V. Chirikov, Statistical properties of a nonlinear string, Sov. Phys. Dokl. 11 (1966) 30.

[3] P. Bocchieri, A. Scotti, B. Bearzi and A. Loinger, Anharmonic chain with Lennard-Jones interaction, Phys. Rev. A 2 (1970) 2013–2018.

[4] E. Diana, L. Galgani, M. Casartelli, G. Casati and A. Scotti, Teor. Mat. Fiz. 29 (1976) 213 [Theor. Math. Phys. 29 (1976) 1022].

[5] M. Casartelli, E. Diana, L. Galgani and A. Scotti, Phys. Rev. A 13 (1976) 1921.

[6] B. Holian, Simulations of Vibrational Relaxation in Dense Molecular Fluids, in: Rendiconti della Scuola Italiana di Fisica "E. Fermi", XCVII Course, eds. G. Ciccotti and W.G. Hoover (North-Holland, Amsterdam, 1986).

[7] R. Livi, M. Pettini, S. Ruffo, M. Sparpaglione and A. Vulpiani, Relaxation to different stationary states in the Fermi–Pasta–Ulam model, Phys. Rev. A 28 (1983) 3544–3552.

[8] R. Livi, M. Pettini, S. Ruffo, M. Sparpaglione and A. Vulpiani, Equipartition thresholds in nonlinear large Hamiltonian systems: the Fermi–Pasta–Ulam model, Phys. Rev. A 32 (1985) 1039–1045.

[9] H. Kantz, Vanishing stability thresholds in the thermodynamic limit of nonintegrable conservative systems, Physica D 39 (1989) 322–335.

[10] M. Pettini and M. Landolfi, Relaxation properties and ergodicity breaking in nonlinear Hamiltonian dynamics, Phys. Rev. A 41 (1990) 768;
M. Pettini and M. Cerruti-Sola, Phys. Rev. A 44 (1991) 975.

[11] C.E. Wayne, Commun. Math. Phys. 103 (1986) 351; 104 (1986) 21; Commun. Math. Phys. 96 (1984) 311, 96 (1984) 331.

[12] G. Benettin, J. Frölich and A. Giorgilli, A Nekhoroshev-type theorem for Hamiltonian Systems with Infinitely Many Degrees of Freedom, Commun. Math. Phys. 119 (1988) 95.

[13] L. Boltzmann, Nature 51 (1895) 413; Lectures on gas theory, translated by S.G. Brush (Univ. of California Press, 1966); see especially section 45, Comparison with experiments.

[14] J.H. Jeans, On the vibrations set up in molecules by collisions, Philos. Mag. 6 (1903) 279; On the partition of energy between matter and aether, Philos. Mag. 10 (1905) 91.

[15] J.E. Littlewood, On the equilateral configuration in the restricted problem of three bodies, Proc. London Math. Soc. (3) 9 (1959) 343–372; the Lagrange configuration in celestial mechanics, Proc. London Math. Soc. (3) 9 (1959) 525–543.

[16] N.N. Nekhoroshev, Exponential estimate of the stability time of near-integrable Hamiltonian systems, Russ. Math. Surv. 32 No. 6 (1977) 1–65; Exponential estimate of the stability time of near-integrable Hamiltonian systems, II, Trudy Sem. Petrovs. No. 5 (1979) 5–50 [in Russian];
G. Benettin, L. Galgani and A. Giorgilli, A proof of Nekhoroshev's theorem for the stability times in nearly integrable Hamiltonian systems, Cel. Mech. 37 (1985) 1–25;
G. Benettin and G. Gallavotti, Stability of motion near resonances in quasi integrable Hamiltonian systems, J. Stat. Phys. 44 (1986) 293–338;
G. Gallavotti, Quasi-integrable mechanical systems, in: Les Houches, Session XLIII, eds. K. Osterwalder and R. Stora (1984).

[17] G. Benettin and A. Tenenbaum, Ordered and stochastic behavior in a two-dimensional Lennard-Jones system, Phys. Rev. A 28 (1983) 3020.

[18] G. Benettin, L. Galgani and A. Giorgilli, Exponential law for the equipartition times among translational and vibrational degrees of freedom, Phys. Lett. A 120 (1987) 23–27.

[19] G. Benettin, L. Galgani and A. Giorgilli, Realization of holonomic constraints and freezing of high frequency degrees of freedom in the light of classical perturbation theory, part I, Commun. Math. Phys. 113 (1987) 87–103; Realization of holonomic constraints and freezing of high frequency degrees of freedom in the light of classical perturbation theory, part II, Commun. Math. Phys. 121 (1987) 557–601.

[20] A. Giorgilli, Rigorous results on the power expansions for integrals of a Hamiltonian system near an elliptic equilibrium point, Ann. Inst. H. Poincaré 48 (1988) 423–439.

[21] E. Diana, L. Galgani, A. Giorgilli and A. Scotti, On the direct construction of integrals of a Hamiltonian system near an equilibrium point, Boll. Unione Mat. It. 11 (1975) 84–89.

[22] G. Benettin, L. Galgani and A. Giorgilli, Boltzmann's ultraviolet cutoff and Nekhoroshev's theorem on Arnold diffusion, Nature 311 (1984) 444.

[23] L. Galgani, Relaxation Times and the Foundations of Classical Statistical Mechanics in the Light of Modern Perturbation Theory, lectures given at the Noto School "Non-Linear Evolution and Chaotic Phenomena", eds. G. Gallavotti and A.M. Anile (Plenum Press, New York, 1988).