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Distribution of characteristic exponents in the thermodynamic limit

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Abstract. The existence of the thermodynamic limit for the spectrum of the Lyapunov characteristic exponents is numerically investigated for the Fermi-Pasta-Ulam β model. We show that the shape of the spectrum for energy density well above the equipartition threshold ε_c allows the Kolmogorov-Sinai entropy to be expressed simply in terms of the maximum exponent $\bar{\lambda}_{max}$. The presence of a power-law behaviour ε^{β} is investigated. The analogies with similar results obtained from the dynamics of symplectic random matrices seem to indicate the possibility of interpreting chaotic dynamics in terms of some 'universal' properties.

1. Introduction

The existence of a thermodynamic limit for the statistical properties of a generic dynamical system is an interesting open problem (Ruelle 1978). Even more difficult, from an analytical point of view, is the problem of how fast this limit is reached and, eventually, the computation of corrections.

For Hamiltonian systems there exists (on the basis of a series of numerical experiments (Benettin *et al* 1980b, Livi *et al* 1985)) the suspicion that some asymptotic behaviours are already obtained with a small number of degrees of freedom N. For instance the stochasticity and the equipartition thresholds in the energy density ε appear to converge already for $N \sim 20$-40.

Recently Ruelle (1982) has discussed the possible existence of a large volume limit of the distribution of characteristic exponents in conservative and dissipative dynamical systems, and obtained simple scaling laws for an intermittent model of turbulence (Frisch *et al* 1978). The possible existence of a limit of a quantity whose definition is close to that of maximum characteristic exponent as $N \to \infty$ has already been proposed by Casartelli *et al* (1976) on the basis of numerical results. Moreover some numerical computations on the one-dimensional equation of Kuramoto-Sivashinsky (Pomeau *et al* 1984, Manneville 1983) show that a limiting distribution in a dissipative case is reached for $\sim$50-100 degrees of freedom.

The numerical measurement of the Lyapunov spectrum (LS) for a Hamiltonian system is of extreme importance, not only to control the thermodynamic limit, but also because of Pesin's relation which connects the distribution of exponents to the Kolmogorov-Sinai (KS) entropy and, therefore, to the rate of production of information (Pesin 1976). We have chosen to measure the distribution of exponents for the

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Fermi-Pasta-Ulam (FPU) β model (Fermi *et al* 1955), where a quite precise determination of the equipartition energy threshold ε_c is known (Livi *et al* 1985). Above the threshold the whole phase space, except for a set of 0 measure, is connected and the exponents do not depend on the initial position in the phase space, thus simplifying the application of Pesin's relation. We obtain a limit distribution for $N \sim 40$–80 which turns out to be a straight line for large values of the energy density. As a consequence, in this region, the KS entropy is proportional to the maximum Lyapunov exponent $\lambda_{\max}$, to be intended as the starting point of the distribution in the thermodynamic limit. The onset of a power-law behaviour of the maximum exponent near the threshold (where the distribution is no more a straight line) is finally observed in analogy with the results of Rechester *et al* (1979) and Benettin (1984) on low-dimensional systems. Similar results have been obtained on symplectic random matrices by Paladin and Vulpiani (1986).

Computations have been performed partly on a Cray-1 computer and partly on a VAX-11/780 computer with 16 digit precision.

In § 2 the FPU β model is introduced and its statistical and dynamical properties are discussed. In § 3 the definition of distribution of characteristic exponents is given and the numerical results are proposed. Section 4 is devoted to conclusions and perspectives.

2. The Fermi–Pasta–Ulam β model

The model represents the dynamics of a chain of N non-linearly coupled oscillators. Its Hamiltonian is

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{(x_i - x_{i+1})^2}{2} + V(x_i - x_{i+1}) \tag{2.1}$$

where the $\{x_i\}$ are the displacements with respect to equilibrium positions and the $\{p_i\}$ are the corresponding conjugate momenta. In the case of the FPU β model the non-linear interaction potential is given, suitably scaling positions and momenta, by

$$V(\xi) = \tfrac{1}{12}\xi^4. \tag{2.2}$$

The Hamilton equations are therefore

$$\begin{aligned} \dot{x}_i &= p_i \\ \dot{p}_i &= (x_{i+1} - 2x_i + x_{i-1}) + \tfrac{1}{3}[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3] \equiv F(\{x_i\}). \end{aligned} \tag{2.3}$$

We always fix periodic boundary conditions $x_1 = x_{N+1}$ while the initial conditions are randomly chosen with the constraint $\Sigma_i p_i(0) = 0$, in order to avoid systematic growth of spatial variables.

The numerical integration has been performed by means of the Verlet (leap-frog) algorithm (Verlet 1967) which preserves the symplectic structure of the Hamiltonian flow, giving a good stability at long times

$$\begin{aligned} x_i(t+\Delta t) &= x_i(t) + p_i(t) \\ p_i(t+\Delta t) &= p_i(t) + \Delta t^2 F(\{x_i(t+\Delta t)\}). \end{aligned} \tag{2.4}$$

Δt is chosen in the range 0.01–0.05 in order to guarantee a conservation of energy of the order of 0.1%. The dependence of the results on the chosen time step has always been kept under control.

At large energy densities ε ($\varepsilon = E/N$) this model is known to exhibit equipartition of the energy among the degrees of freedom. Livi *et al* (1985) introduced an indicator in the Fourier space, the spectral entropy, which clearly reveals the existence of a threshold at $\varepsilon = \varepsilon_c \simeq 0.1$ with the present scale. In the equipartiton region the phase space is likely to be connected: this is confirmed by some measurements performed for different initial conditions at the same energy density.

The trajectories are chaotic and all the Lyapunov exponents are different from zero (apart from the four which are zero due to energy and momentum conservation, see § 3), even if long relaxation times of mean values and characteristic exponents are still observed. Below the critical value ε_c, the Lyapunov exponents in general depend on the initial conditions and intriguing 'branching phenomena' can occur. Thus we do not enter this region where a LS is not unequivocally defined.

3. Lyapunov exponents distribution: numerical results

The Lyapunov characteristic exponents naturally derive from the extension of the linear stability analysis to aperiodic motion. As is well known, they measure the average exponential divergence from a given trajectory when the initial condition is perturbed with respect to preassigned directions. For a dynamical system characterised by $2N$ degrees of freedom one can define

$$\Lambda(\boldsymbol{e}, N) = \lim_{t\to\infty} \frac{1}{t} \ln\|L_t \boldsymbol{e}\| \tag{3.1}$$

where L_t is the linear mapping associated with the flow, $\|\cdot\|$ represents the Euclidean norm in $\mathbb{R}^{2N}$ and $\boldsymbol{e}$ is a generic vector in the tangent space. The dependence of Λ on the initial condition has, instead, been neglected, since we are interested here in analysing the region above the equipartition threshold of the model (2.1).

It can be easily proven that, when $\boldsymbol{e}$ is varied, $\Lambda(\boldsymbol{e}, N)$ takes $2N$ different values $\Lambda_1(N) > \Lambda_2(N) > \ldots > \Lambda_{2N}(N)$, which constitute the so-called LS. The very definition of LS is, however, impractical for numerical applications because almost any choice of $\boldsymbol{e}$ would yield the same limit value $\Lambda_1(N)$.

A different approach (see Benettin *et al* 1980*a*), based on the expansion rates of p-dimensional subspaces

$$\chi_p = \lim_{t\to\infty} \frac{1}{t} \ln\|L_t\boldsymbol{e}_1 \wedge L_t\boldsymbol{e}_2 \wedge \ldots \wedge L_t\boldsymbol{e}_p\| \tag{3.2}$$

has to be applied, where $(\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_p)$ represents a basis of a p-dimensional subspace. Indeed it has been proven (Benettin *et al* 1980a, b) that

$$\chi_p(N) = \sum_{i=1}^{p} \Lambda_i(N). \tag{3.3}$$

This provides a basis for defining a numerical algorithm. In fact one can randomly choose an orthonormal basis in the tangent space and let it evolve in time. The Gram-Schmidt orthogonalisation procedure can then be applied at fixed time intervals. This simultaneously allows the evaluation of the partial expansion rates and avoids the angles among the vectors $L_t\boldsymbol{e}_i$ becoming too small.

The existence of a finite thermodynamic limit for the LS simply means that the quantity $\Lambda_{\alpha N}(N) \equiv \lambda(\alpha, N)$ is independent of N for large N (and N/V constant, where V is the volume occupied by the dynamical system) and an asymptotic spectrum $\tilde{\lambda}(\alpha)$ can be defined

$$\tilde{\lambda}(\alpha) = \lim_{N \to \infty} \lambda(\alpha, N).$$

In particular, by this definition, the value $\tilde{\lambda}(0)$ will correspond to the maximum Lyapunov characteristic exponent, and, from here on, will be indicated by $\tilde{\lambda}_{\max}$.

As far as Hamiltonian systems are concerned it can be proven that, as a consequence of their symplectic structure, Lyapunov exponents exist in pairs with opposite values ($\Lambda_i = -\Lambda_{2N+1-i}$). Moreover one has as many null Lyapunov characteristic exponents as the double of the constants of motion in involution. Anyway, the interest in studying the LS of a Hamiltonian system like (2.1) comes from Pesin's theorem, which connects $\lambda(\alpha, N)$ with the Kolmogorov–Sinai entropy h (i.e. the rate of creation of information) of the system; in formulae

$$h(N) = \sum_{i=1}^{N} \lambda\left(\frac{i}{N}, N\right). \tag{3.4}$$

As a consequence of (3.4), we shall limit ourselves to analysing the positive part of the LS (PLS).

Let us observe that, due to the periodic boundary conditions, there exists a second integral of motion (momentum) besides energy, thus leading to two null exponents in the PLS.

Now we want to investigate numerically the existence of the thermodynamic limit for the PLS of the FPU β model defined in (2.1) and then, if this is the case, obtain an estimate for $h(N)$.

For this purpose we have varied N at fixed ε; in figure 1 we have reported the PLS for $\varepsilon = 26.4$. Such energy density ε is much greater than the critical value ε_c so that the $\lambda(\alpha, N)$ are sufficiently high for almost any α to obtain a fast convergence to their asymptotic values. This limited the integration times of the equations of motion below $t \sim 10^4$.

First of all let us observe that the numerical results show the evidence of a limit distribution as N increases: the thermodynamic limit is practically reached for $N \sim$ 20–40.

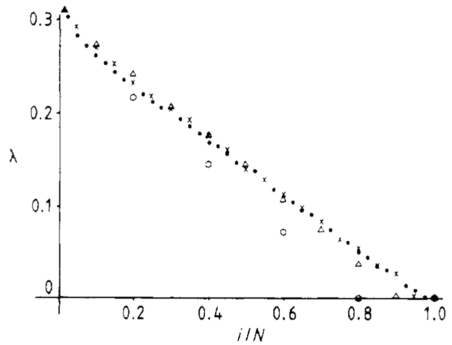

Figure 1. $\lambda(i/N, N)$ plotted against i/N for different values of N (○, 5; △, 10; ×, 20; ●, 40; ▲, 80) and $\varepsilon = 26.4$.

Moreover, as a verification of the correctness of our results, in all the PLS that we have reported, the exponents Λ_N and Λ_{N-1} are zero ($\leqslant 10^{-4}$) as we expected. But, what one could not *a priori* expect is that the shape of the asymptotic (read thermodynamic limit) PLS is linear in a wide range, except near $\tilde{\lambda}_{max}$, where it tends to enhance. To clarify this point we have performed further numerical analysis varying ε, and pointing our attention to the distribution close to $\tilde{\lambda}_{max}$. Figure 2 shows the interesting part of the PLS for $\varepsilon = 3.58$ and $N = 40$ and 80. Again in this case the two distributions overlap in the intermediate linear region, while some small deviation is observed around $\alpha = 0$. This behaviour suggests that as ε is lowered, the convergence to the thermodynamic limit is slower, at least in the $\tilde{\lambda}_{max}$ region. Anyway, no major change in the shape of the distribution is observed. To obtain a clearer understanding of the approach to the thermodynamic limit of the PLS we have studied how $\lambda(\alpha, N)$ varies with N, for fixed α. Once the energy density is chosen $\varepsilon = 1$, the exponent $\lambda(0.05, N)$ has been evaluated for chains composed of $N = 20$, 40, 80 and 160 particles (see figure 3). Although the poor statistics (due to unfeasibility of measurements at larger values of N) one can conclude that the convergence is not monotonic, and one cannot exclude an oscillating behaviour around the asymptotic value which we interpret as the value of $\tilde{\lambda}(0.05)$ in the thermodynamic limit. Now let us discuss an interesting consequence of the straight line behaviour of the asymptotic PLS for sufficiently high energy densities.

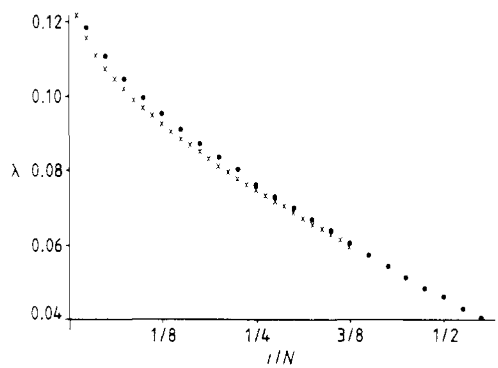

Figure 2. The upper part of the PLS for $N = 40$ (●), 80 (×) and $\varepsilon = 3.58$.

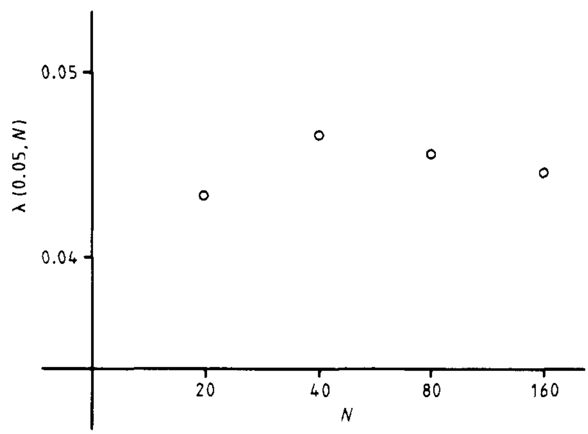

Figure 3. $\lambda(0.05, N)$ plotted against N for $\varepsilon = 1$.

The linearity of $\tilde{\lambda}(\alpha)$ simply means that for large N the density $\rho(\tilde{\lambda})$ of characteristic exponents in the interval $(\tilde{\lambda}, \tilde{\lambda}+\mathrm{d}\tilde{\lambda})$ is constant, namely

$$\rho(\tilde{\lambda}) = CN \qquad \tilde{\lambda} < \tilde{\lambda}_{\max} \tag{3.5}$$

where C is independent not only of $\tilde{\lambda}$ but also of N, due to the existence of a thermodynamic limit. Now from the definition of $\rho(\tilde{\lambda})$ one obtains the relation

$$N = \int_0^{\tilde{\lambda}_{\max}} \rho(\tilde{\lambda})\, \mathrm{d}\tilde{\lambda} = CN\tilde{\lambda}_{\max} \tag{3.6}$$

yielding

$$C = 1/\tilde{\lambda}_{\max}. \tag{3.7}$$

This allows us to obtain by a straightforward calculation (see equation (3.4)) the h of the system as a function of $\tilde{\lambda}_{\max}$ only:

$$h = \int_0^{\tilde{\lambda}_{\max}} \tilde{\lambda} CN \, \mathrm{d}\tilde{\lambda} = \tfrac{1}{2} N \tilde{\lambda}_{\max}. \tag{3.8}$$

This relation provides a recipe to obtain, at fixed ε, a numerical estimate of the entropy density of the FPU β model in the thermodynamic limit, simply extrapolating the distribution obtained for a sufficiently high value of N to determine $\tilde{\lambda}_{\max}$. For low ε this recipe instead provides only an upper bound of this quantity, because, as we have shown, the distribution tends to enhance around $\alpha = 0$. Anyway, the existence of a finite limit of $\tilde{\lambda}_{\max}$ is still well verified for $\varepsilon = 1$ since the estimate of $\tilde{\lambda}_{\max}$ obtained by a fit of the PLS turned out to be stable for increasing N: figure 4 in fact shows that $\lambda(1/320, 320)$ falls on the fit of the limit PLS obtained for $N = 80$ and 160.

It is also relevant to study how $\tilde{\lambda}_{\max}$ scales with ε. To this end we have chosen $N = 80$ (this guarantees obtaining the limit PLS in the chosen range of energy densities) and we have fitted the distribution of the first five exponents with the function

$$\tilde{\lambda}(\alpha) = a/(b+\alpha) \tag{3.9}$$

which seems to be sufficiently accurate in describing the PLS near $\alpha = 0$. Figure 5 shows that for high values of ε the dependence tends to weaken, while for small ε the onset

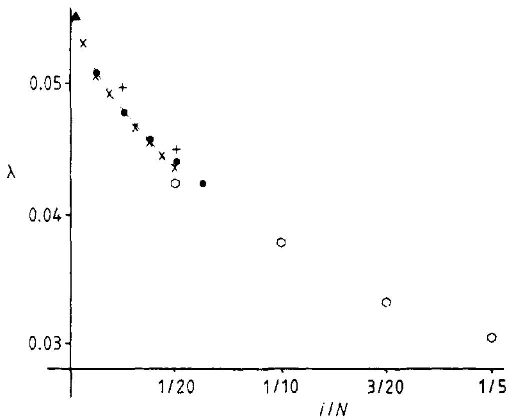

Figure 4. The upper part of the PLS for the different N (○, 20; +, 40; ●, 80; ×, 160; ▲, 320) and $\varepsilon = 1$. The broken curve represents the fit obtained by (3.9) for $N = 160$.

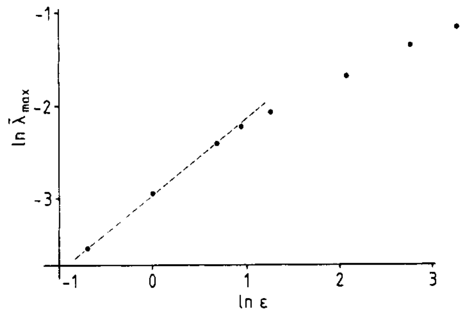

Figure 5. $\ln \lambda_{max}$ as a function of $\ln \varepsilon$ for $N = 80$. The broken curve has been drawn to guide the eyes to the power-law behaviour.

of a power-law behaviour $\tilde{\lambda}_{max} \sim \varepsilon^{\beta}$ can be reasonably assumed, with $\beta \simeq 0.78$. Even if it is extremely hard to investigate in more detail the small ε region because of computer time limitations, it is however interesting to underline the analogies with the results of Benettin (1984) and Rechester *et al* (1979) who found $\beta = \frac{1}{2}$ and $\frac{2}{3}$ in low-dimensional systems.

Finally it is worthwhile noticing the monotonously decreasing behaviour of the parameter b when the energy ε is decreased. This indeed confirms the previously sketched tendency of $\tilde{\lambda}(\alpha)$ to squeeze against the λ axis for small ε values. A quantitative analysis is however quite involved in the absence of any analytic ansatz on the behaviour of $\tilde{\lambda}(\alpha)$ for small α.

4. Conclusions

The major result of the present paper concerns the existence of the thermodynamic limit for the LS with a special reference to the finiteness of $\tilde{\lambda}_{max}$. Indeed, it is not at all *a priori* obvious that the growth of degrees of freedom does not lead to a constantly increasing $\tilde{\lambda}_{max}$. At variance with this naive picture, it must be registered that the average exponential divergence of nearby trajectories is independent of N in the limit of large $N(\sim 40)$.

Moreover the seemingly power-law behaviour of $\tilde{\lambda}_{max}$ against ε suggests, recalling the existence of an equipartition as well as of a stochasticity threshold, the presence of an underlying structure similar to that of phase transitions.

Finally, a few words on the comparison of our results with those obtained by multiplying N-dimensional random symplectic matrices (Paladin and Vulpiani 1986). The straight line behaviour of the LS means that the generating dynamics is not relevant for determining the distribution of characteristic exponents. Only a few still hidden parameters could play a relevant role. We are investigating the latter problem.

After the completion of this paper we were informed by C M Newman that he had obtained an asymptotically uniform distribution of Lyapunov exponents for a continuous-time linear stochastic model (Newman 1986). In view of the results on random symplectic matrices by Paladin and Vulpiani (1986) and on some preliminary results on symplectic maps we think that the existence of an asymptotic distribution and the fact that it is uniform in some region of the parameters (e.g. at large energy densities for the FPU model) is more than a coincidence.

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