

Modulational estimate for the maximal Lyapunov exponent in Fermi-Pasta-Ulam chains

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In the framework of the Fermi-Pasta-Ulam (FPU) model, we show a simple method to give an accurate analytical estimation of the maximal Lyapunov exponent at high energy density. The method is based on the computation of the mean value of the modulational instability growth rates associated to unstable modes. Moreover, we show that the strong stochasticity threshold found in the β -FPU system is closely related to a transition in tangent space, the Lyapunov eigenvector being more localized in space at high energy. [S1063-651X(97)50112-7]

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A large number of theoretical and numerical studies have been devoted to the characterization of chaotic high-dimensional systems, but in spite of these efforts several fundamental items are not yet fully understood. In particular, the relation between Lyapunov analysis and other phase space properties like diffusion of orbits, relaxation to equilibrium states, and spatial development of instability remain to be clarified [1]. This Rapid Communication, besides presenting an estimate of the largest Lyapunov exponent λ_1 , is a contribution to clarify this relationship in the context of the Fermi-Pasta-Ulam (FPU) model [2]. This system was not only the starting point of the (re)discovery of the soliton [3], but initiated also several studies of the mixed chaotic-ordered phase space structure based on resonance overlap criteria [4], KAM theorem and Nekhoroshev stability estimates [5]. Statistical mechanics was also tested on this equation [6,7] and the results showed that ergodicity is not an obvious consequence of the nonexistence of analytical first integrals of motion.

There are very few examples of analytical calculations of λ_1 in the chaotic component corresponding to energy equipartition in high-dimensional systems [8,9]. In this Rapid Communication, we derive an approximate analytical expression for λ_1 that agrees very well with numerical simulations. We focus our attention on the asymptotic state of the system, when it has reached energy equipartition, i.e., the state where energy is evenly distributed among all Fourier modes (relaxation times [10] will not be our concern here). One of the main points of this paper is to emphasize the relevant role played by some unstable periodic orbits corresponding to Fourier modes. Therefore, we will first derive the criterion for modulational instability of a plane wave on the lattice.

Denoting by $u_n(t)$ the position of the n th atom ($n \in [1, N]$), the equations of motion of the FPU chain read

$$\ddot{u}_n = u_{n+1} + u_{n-1} - 2u_n + \beta[(u_{n+1} - u_n)^{2p+1} - (u_n - u_{n-1})^{2p+1}], \quad (1)$$

where p is an integer greater than or equal to 1. We choose periodic boundary conditions. Even if the positive parameter β can be forgotten by appropriate scaling transformations of u_n , we will keep it in order to make reliable comparisons with previous papers, where $\beta=0.1$. For the sake of simplicity, we consider first the case $p=1$ and then we generalize to any p value.

Looking for plane wave solutions

$$u_n(t) = \phi_0(e^{i\theta_n(t)} + e^{-i\theta_n(t)}), \quad (2)$$

where $\theta_n(t) = qn - \omega t$ and $q = 2\pi k/N$, we obtain the dispersion relation $\omega^2(q) = 4(1 + \alpha)\sin^2(q/2)$, where $\alpha = 12\beta\phi_0^2\sin^2(q/2)$ takes into account the nonlinearity [11]. The modulational instability of such a plane wave is investigated by studying the linearized equation associated to the envelope of the carrier wave. Therefore, one introduces an infinitesimal perturbation in the amplitude and looks for solutions:

$$u_n(t) = [\phi_0 + b_n(t)]e^{i\theta_n(t)} + [\phi_0 + b_n^*(t)]e^{-i\theta_n(t)}. \quad (3)$$

Introducing this ansatz in Eq. (1), after linearization with respect to b_n but keeping the second derivative (in contrast to what has been done for Klein-Gordon type equation [12]), we obtain

$$\begin{aligned} \ddot{b}_n - 2i\omega\dot{b}_n = & (1 + 2\alpha)(b_{n+1}e^{iq} + b_{n-1}e^{-iq} - 2\cos(q)b_n) \\ & + \alpha(b_{n+1}^* + b_{n-1}^* - 2\cos(q)b_n). \end{aligned} \quad (4)$$

Assuming further $b_n = Ae^{i(Qn - \Omega t)} + Be^{-i(Qn - \Omega t)}$, we finally obtain the following dispersion relation

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$$\left[(\Omega + \omega)^2 - 4(1 + 2\alpha) \sin^2 \left(\frac{q+Q}{2} \right) \right] \left[(\Omega - \omega)^2 - 4(1 + 2\alpha) \sin^2 \left(\frac{q-Q}{2} \right) \right] = 4\alpha^2 (\cos Q - \cos q)^2. \quad (5)$$

This equation has four different solutions once q (wave vector of the unperturbed wave) and Q (wave vector of the perturbation) are given. If one of the solutions is complex we have an instability of one of the modes ($q \pm Q$) with a growth rate equal to the imaginary part of the solution. Therefore, one can compute the instability threshold for any initial linear wave, i.e., any wave vector and any amplitude. For example, for $q=0$ we find that the solution is obviously stable since the zero mode, corresponding to translation invariance, is completely decoupled from the others. For $q=\pi$, the expression for the growth rate is

$$\tau(\pi, Q) = 2 \left[\sqrt{(1+\alpha)(4+8\alpha)\cos^2(Q/2) + \alpha^2\cos^4(Q/2)} - 1 - \alpha - (1+2\alpha)\cos^2(Q/2) \right]^{1/2}. \quad (6)$$

A simple analysis of this function shows that the first unstable mode is the nearest mode corresponding to $Q=2\pi/N$. Computing the critical value of the parameter α above which $\tau(\pi, 2\pi/N)$ is positive, we obtain the critical energy E_c for the π mode. It reads

$$E_c = \frac{2N}{9\beta} \sin^2 \left(\frac{\pi}{N} \right) \frac{7\cos^2 \left(\frac{\pi}{N} \right) - 1}{\left[3\cos^2 \left(\frac{\pi}{N} \right) - 1 \right]^2}. \quad (7)$$

This analytical expression is in agreement with the previous [13–15] approximate expression $E_c \approx \pi^2/3N\beta$ valid only in the large N limit. Above this energy threshold, the π mode is therefore unstable and gives rise to a chaotic localized breatherlike excitation, able to move very fast in the system, collecting energy from high-wave-vector phonons until its disappearance leads to the final energy equipartition [16].

When the energy increases, the region of instability extends to a larger region of wave vectors, and, in particular, the most unstable mode $\frac{Q_{\max}}{2}$ increases until the asymptotic value $Q_{\max} = 2 \arccos(\sqrt{8/\sqrt{3}-4}) \approx 0.42\pi$ is reached. It is important to notice that, for sufficiently high energy, the rescaled growth rate $\tau/\tau(\pi, Q_{\max})$ does not depend on the energy density. The growth rate is plotted in Fig. 1 at high energy.

We performed some simulations of the system using a sixth-order symplectic integration scheme adopting as initial condition the π mode and computing, after the transition to equipartition, the Lyapunov exponents with the standard method by Benettin *et al.* [17]. The results are plotted in Fig. 2.

Let us present now the analytical estimation of λ_1 . As the system is symplectic, the usual pairing rule is valid and, moreover, Pesin's theorem allows us to identify the Kolmogorov-Sinai entropy of the system with the sum of all positive Lyapunov exponents. As the spectrum was shown

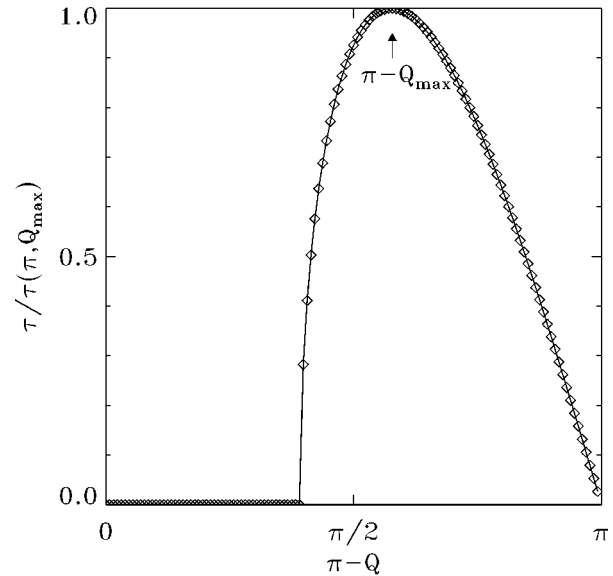


FIG. 1. Shape of the growth rate $\tau(\pi, Q)/\tau(\pi, Q_{\max})$ for sufficiently high energy. The diamonds correspond to the case $N=256$ and the solid curve to the asymptotic shape when N goes to infinity.

[18] to be approximately linear at high energy (see the inset of Fig. 2), one can relate the Kolmogorov-Sinai entropy S_{KS} with λ_1 . Namely,

$$S_{\text{KS}} = \sum_{i=1}^N \lambda_i \approx \lambda_1 N/2. \quad (8)$$

Let us define the instability entropy

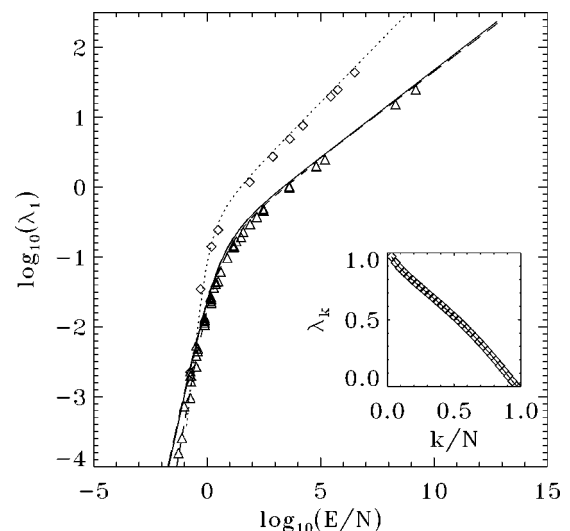


FIG. 2. Comparison of the analytical estimate with numerical data for the maximal Lyapunov exponent λ_1 . The solid curve corresponds to our estimation [Eq. (10)], the dashed curve to the estimate of Ref. [9] and the triangles to our numerical results (for the β -FPU, i.e., $p=1$). The dotted curve (diamonds) corresponds to the analytical estimate (numerical results) in the case of a power $p=2$. In the inset, we plot the N positive Lyapunov in the case $E/N=4200$ and $p=1$.

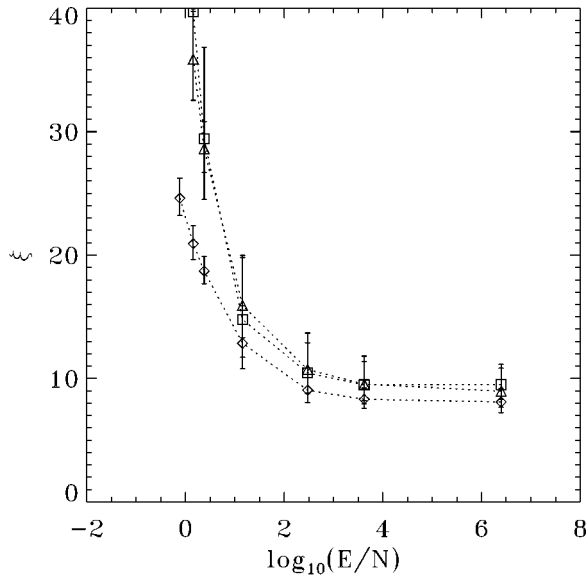


FIG. 3. Participation ratio ξ vs the density of energy E/N , for different lattice sizes; diamonds for $N=64$, triangles for $N=256$, and squares for $N=1024$.

$$S_{\text{IE}}(q) = \sum_{i=1}^{N/2} \tau(q, 2\pi i/N), \quad (9)$$

where the sum is over all positive growth rates [19]. The crucial physical hypothesis of this paper is that $S_{\text{KS}} \approx S_{\text{IE}}(\pi)$, we then obtain the following analytical expression for the maximal Lyapunov exponent:

$$\lambda_1 = \frac{2}{N} \sum_{i=1}^{N/2} \tau(\pi, 2\pi i/N), \quad (10)$$

where the τ expression is given in Eq. (6). Figure 2 attests that the analytical estimate (10) is very accurate. In the same figure the data obtained with a Riemannian differential geometrical approach, developed in [9], are also shown. The two methods give almost identical results, apart at very low energy, where the findings of Ref. [9] are in better agreement with our numerical data.

It is remarkable to note that Chirikov [20] found similarly the maximal Lyapunov exponent of the standard map at high energy by averaging over the phase space the maximal eigenvalue associated to the main hyperbolic point. It corresponds in our case to averaging the growth rate (6) for the unstable periodic orbit $q = \pi$ over the equilibrium equipartition state (where all modes have the same weight). A similar approach is known as Toda criterion [21] and although it cannot be used as a signature of chaos, it can give an approximate estimation of λ_1 . On the other hand, it is known that crude stochastic approximations can give good estimates of λ_1 also for high-dimensional strongly chaotic symplectic systems [22].

In fact, one can understand average (10) in a better way by recalling that the modes $\{\pi/2\}, \{2\pi/3\}, \{\pi\}$ correspond to the simplest unstable periodic orbits and are also the only three one-mode solutions of the β -FPU problem. The calculation of the instability entropies of these three modes shows that they are extremely close to one another, in contrast to

the value for other modes. A correct approach would be to apply the ζ -function formalism [23] to this system, if feasible.

At high energy, expression (6) can be simplified as $\tau(\pi, Q) \approx \sqrt{\alpha} f(Q)$, where $f(Q)$ is energy independent. Therefore, the growth rate scales with the amplitude ϕ_0 , and as $E = N(8\phi_0^2 + 64\beta\phi_0^4)$, it means that the growth rate and, therefore, λ_1 scales with $(E/N)^{1/4}$ at high energy. This result is in contradiction with Ref. [24] but in agreement with Ref. [9].

In fact, a similar approach gives also very good results for other powers $2(p+1)$ in the coupling potential. The expression of the growth rate is then the same if we use $\alpha = \beta((2p+1)!/p!(p+1)!(2\phi_0 \sin(q/2))^{2p}$. Figure 2 shows that the results are once more in very good agreement with numerical estimates. One derives easily that the maximal Lyapunov scales at high energy like $\lambda_1 \sim (E/N)^{1/2 - [1/2(p+1)]}$. It is important to stress that in the limit of hard potential ($p \rightarrow \infty$) we find the exponent 1/2, analogously to billiards [25]. In the low energy limit, however, all models have the same scaling behaviors as expected.

Plotting $\lambda_1(E/N)$ in a log-log scale we observe (see Fig. 2) that the two asymptotic linear behaviors are separated by a “knee” (change in slope) at intermediate energy density. An estimation of this transition region can be derived assuming that the linear and nonlinear contributions to $\omega(q)$ should be of the same order. We obtain $\alpha \sim 1$, i.e., an energy density of the order of $1/\beta$ (this is equivalent to the estimation given by mode overlap criterion [4]).

This knee corresponds to a stochasticity threshold [7] that defines the crossing from weak to strong chaos. But we have also found that it corresponds to an interesting transition in tangent space. Considering the normalized Lyapunov vector V_1 associated to the maximal Lyapunov λ_1 , we can introduce the participation ratio [26]

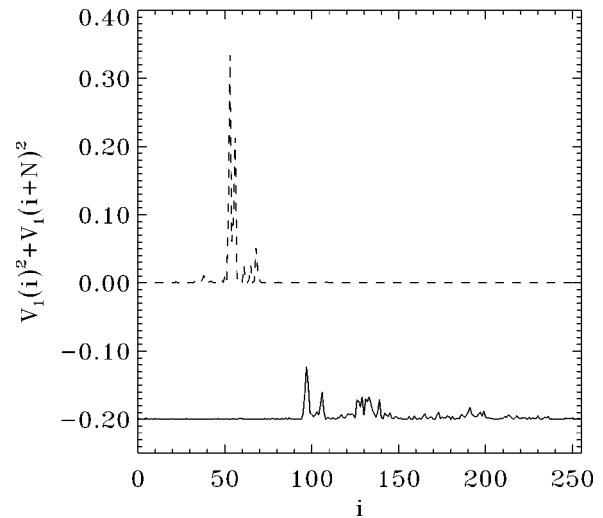


FIG. 4. Localization in tangent space of the Lyapunov vector for $N=256$. The dashed curve corresponds to a generic localized Lyapunov vector at high energy density $E/N \approx 2.5 \times 10^6$, whereas the solid curve (shifted by -0.2) corresponds to a generic delocalized one at low energy density $E/N \approx 2$.

$$\xi = \left(\sum_{i=1}^N [V_1(i)^2 + V_1(i+N)^2]^2 \right)^{-1}, \quad (11)$$

where the first (last) N components of V_1 are associated to the evolution of linear perturbation of u_n (\dot{u}_n) in tangent space. The quantity (11) has been used in different contexts and, for example, in dynamical systems [27] as an indicator of localization: it is of order N if the vector is extended and of order one if localized. We have found that the stochasticity threshold corresponds to a crossover from an extended state in tangent space to a more localized state, as attested by Fig. 3. The two examples of Lyapunov vectors reported in Fig. 4 show the clear difference between low and high energy density. The localization of the Lyapunov vectors for chains of nonlinear oscillators in the high energy limit was also previously observed in Refs. [8,28]. Moreover, signatures of a similar transition were found in [22] for a model of coupled symplectic maps. Finally, we notice that the metallic-insulating transition in finite samples [29] is very reminiscent of the one reported in this Communication.

We conclude by stressing again that we have computed the maximal Lyapunov for a high dimensional Hamiltonian system by using a simple analytical approach, based upon modulation instability analysis of linear waves. The results obtained here are in excellent agreement with our computer simulation results. The success of this calculation suggests that this Lyapunov estimation could be extended to other high-dimensional Hamiltonian systems. Moreover, we have shown that the strong stochasticity threshold [7] is *not* a threshold to energy equipartition, since equipartition can be always obtained, although on longer time scales [30]. It rather corresponds to a crossover from extended to more localized states in tangent space.

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