

Analytical estimation of the maximal Lyapunov exponent in oscillator chains

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February 27, 1998

Abstract

An analytical expression for the maximal Lyapunov exponent λ_1 in generalized Fermi-Pasta-Ulam oscillator chains is obtained. The derivation is based on the calculation of modulational instability growth rates for some unstable periodic orbits. The result is compared with numerical simulations and the agreement is good over a wide range of energy densities ε . At very high energy density the power law scaling of λ_1 with ε can be also obtained by simple dimensional arguments, assuming that the system is ruled by a single time scale. Finally, we argue that for repulsive and hard core potentials in one dimension $\lambda_1 \sim \sqrt{\varepsilon}$ at large ε .

1 INTRODUCTION

Many theoretical and numerical studies have been devoted to the characterization of chaos in high-dimensional systems. Nevertheless, several fundamental issues are not understood. In particular, the relation between Lyapunov instability analysis and phase space properties like diffusion of orbits, relaxation to equilibrium states, spatial development of instabilities remains to be clarified (see Ref. [1] for a review).

In this paper we present an analytical estimate of the largest Lyapunov exponent λ_1 of the Fermi-Pasta-Ulam (FPU) model [2] based on the study of modulational instabilities of linear waves. The FPU model has played for dynamical system theory a similar role to the Ising model in statistical mechanics. Let's just quote some major studies and discoveries motivated by the FPU numerical experiment: the introduction of the concept of soliton [3], the prediction of the transition to large-scale chaos by the resonance overlap criterion [4], the use of KAM perturbation theory and Nekhoroshev stability estimates [5], the numerical detection of the strong stochasticity threshold [6].

Some attempts already exist [7, 8] of computing analytically λ_1 in the FPU model. Here we present a completely different approach, which emphasizes the relevant role played by some unstable periodic orbits related to the representation in Fourier modes [9] (preliminary results were already presented in Ref. [10]).

In the present contribution, our analysis will be limited to the asymptotic state, where energy is equally shared among all normal modes. In Sect. 2, the modulational instability of a plane wave on the lattice is discussed, while in Sect. 3 an approximate analytical expression for λ_1 is obtained from

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the growth rates of the modulational instability, and is compared with numerical results. Finally, in Sect. 4 it is shown that, for sufficiently high energy density ε , the dynamics of the system, in the phase as well as in the tangent space, is ruled by a single time scale $\tau(\varepsilon)$ and some extensions of the results to repulsive and hard core systems are presented.

2 MODULATIONAL INSTABILITY ANALYSIS

Denoting by $u_n(t)$ the position of the n -th atom ($n \in \{1, \dots, N\}$), the equations of motion for the generalized FPU chain read

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

where p is an integer with $p \geq 1$, the parameter β is fixed to 0.1 for comparison with previous results and periodic boundary conditions have been adopted. For sake of simplicity, we first report the analysis for $p = 1$ (i.e. for the usual β -FPU model) and then we generalize the results to any p -value. Due to the periodic boundary conditions, the normal modes associated to the linear part of Eq. (1) are plane waves of the form

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

where $\theta_n(t) = qn - \omega t$ and $q = 2\pi k/N$. The dispersion relation is $\omega^2(q) = 4(1 + \alpha) \sin^2(q/2)$, 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 (2). Therefore, one introduces infinitesimal perturbations in the amplitude and phase and looks for solutions

$$\begin{aligned} u_n(t) &= \phi_0 [1 + b_n(t)] e^{i[\theta_n(t) + \psi_n(t)]} + \phi_0 [1 + b_n(t)] e^{-i[\theta_n(t) + \psi_n(t)]} \\ &= 2\phi_0 [1 + b_n(t)] \cos[qn - \omega t + \psi_n(t)] \end{aligned} \quad (3)$$

where b_n and ψ_n are assumed to be small in comparison with the parameters of the carrier wave. Substituting Eq. (3) into the equations of motion and keeping the second derivative (at variance with what has been done for Klein-Gordon type equation [12, 13]), we obtain for the real and imaginary part of the secular term $e^{i(qn - \omega t)}$

$$\begin{aligned} -\omega^2 b_n + 2\omega \dot{\psi}_n + \ddot{b}_n &= (1 + 2\alpha) [\cos q (b_{n+1} + b_{n-1}) - 2b_n] \\ &\quad - \alpha (b_{n+1} + b_{n-1} - 2b_n \cos q) - (1 + 2\alpha) \sin q (\psi_{n+1} - \psi_{n-1}) \end{aligned} \quad (4)$$

$$\begin{aligned} -\omega^2 \psi_n - 2\omega \dot{b}_n + \ddot{\psi}_n &= (1 + 2\alpha) [\cos q (\psi_{n+1} + \psi_{n-1}) - 2\psi_n] \\ &\quad + (1 + 2\alpha) \sin q (b_{n+1} - b_{n-1}) + \alpha (\psi_{n+1} + \psi_{n-1} - 2\psi_n \cos q) \end{aligned} \quad (5)$$

Assuming further $b_n = b_0 e^{i(Qn - \Omega t)} + \text{c.c.}$ and $\psi_n = \psi_0 e^{i(Qn - \Omega t)} + \text{c.c.}$ we obtain the two following equations for the secular term $e^{i(Qn - \Omega t)}$

$$b_0 \left[\Omega^2 + \omega^2 + 2(1 + 2\alpha)(\cos q \cos Q - 1) - 2\alpha(\cos Q - \cos q) \right] - 2i\psi_0 [\omega\Omega + (1 + 2\alpha) \sin q \sin Q] = 0 \quad (6)$$

$$\psi_0 \left[\Omega^2 + \omega^2 + 2(1 + 2\alpha)(\cos q \cos Q - 1) + 2\alpha(\cos Q - \cos q) \right] + 2ib_0 [\omega\Omega + (1 + 2\alpha) \sin q \sin Q] = 0 \quad (7)$$

Non trivial solution for (b_0, ψ_0) are found only if the determinant vanishes, i.e. if the following equation is fulfilled:

$$\begin{aligned} \left[(\Omega + \omega)^2 - 4(1 + 2\alpha) \sin^2 \left(\frac{q + Q}{2} \right) \right] &\quad \left[(\Omega - \omega)^2 - 4(1 + 2\alpha) \sin^2 \left(\frac{q - Q}{2} \right) \right] \\ &= 4\alpha^2 (\cos Q - \cos q)^2 \end{aligned} \quad (8)$$

This equation admits 4 different solutions once q (wavevector of the unperturbed wave) and Q (wavevector of the perturbation) are fixed. 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 derive the instability threshold for any initial linear wave, i.e. any wavevector and any amplitude.

For example, for $q = 0$, we obtain $\Omega = \pm \sin(Q/2)$, which proves that the solution is obviously stable since the zero-mode, corresponding to translation invariance, is completely decoupled from the others.

For $q = \pi$, one can easily see that Eq. (8) admits two real and two imaginary solutions if and only if

$$\cos^2 \frac{Q}{2} > \frac{1 + \alpha}{1 + 3\alpha} \quad (9)$$

Being $\alpha = 12\beta\phi_0^2 = 3\beta(2\phi_0)^2 = 3\beta a^2$ (where $a = 2\phi_0$), this formula is equivalent to the formula found by Sandusky and Page [14]. Moreover, it can be easily shown that the first unstable mode, associated to the perturbation, corresponds to $Q = 2\pi/N$ and therefore the critical amplitude a_c above which the π -mode loses stability is:

$$a_c = \left[\frac{\sin^2 \left(\frac{\pi}{N} \right)}{3\beta \left[3 \cos^2 \left(\frac{\pi}{N} \right) - 1 \right]} \right]^{1/2} \quad (10)$$

Since for the π -mode the energy is simply given by $E = N(2a^2 + 4\beta a^4)$, we finally get the critical energy

$$E_c = \frac{2N}{9\beta} \sin^2 \left(\frac{\pi}{N} \right) \frac{7 \cos^2 \left(\frac{\pi}{N} \right) - 1}{\left[3 \cos^2 \left(\frac{\pi}{N} \right) - 1 \right]^2} \quad (11)$$

For large values of N , we obtain, in agreement with previous approximate estimations [9, 15, 16], the expression

$$E_c = \frac{\pi^2}{3\beta N} + O \left(\frac{1}{N^3} \right). \quad (12)$$

that turns out to be quite accurate for $N > 50 - 60$. Above this energy threshold, the π -mode is therefore unstable and gives rise to a “chaotic breather”, that has a finite life-time and finally disappears leading to energy equipartition (this complex relaxation process to equipartition is described in detail in Ref. [17]).

3 GROWTH RATES AND LYAPUNOV EXPONENTS

Again for the π -mode, from Eq. (8), one can compute the growth rate $\sigma(\pi, Q) = \text{Im}(\Omega(Q))$ from Eq. (8)

$$\sigma(\pi, Q) = 2\sqrt{\sqrt{4(1 + \alpha)(1 + 2\alpha) \cos^2 \frac{Q}{2} + \alpha^2 \cos^4 \frac{Q}{2} - 1 - \alpha - (1 + 2\alpha) \cos^2 \frac{Q}{2}}} \quad (13)$$

It is plotted in Fig. 1 for two different amplitudes. When the amplitude (or energy density) increases, the region of instability extends to a larger region of wavevectors, and in particular the most unstable mode Q_{\max} increases reaching an asymptotic value $\tilde{Q}_{\max} = 2 \arccos \left(\sqrt{\frac{8}{\sqrt{3}} - 4} \right) \simeq 0.42\pi$. It is important to notice that, for sufficiently high energy, the rescaled growth rate $\sigma/\sigma(\pi, Q_{\max})$ does not depend on the energy density. This suggests that in the high energy limit a unique time scale is present in the system; we will discuss in more detail this point in the following.

One can also derive the lowest unstable mode, whose asymptotic limit at high energy is $\tilde{Q}_{\min} = 2 \arccos(1/\sqrt{3}) \simeq 0.6\pi \simeq 1.91$ (as previously derived in [9]). Fig. 2 reports the stability and instability

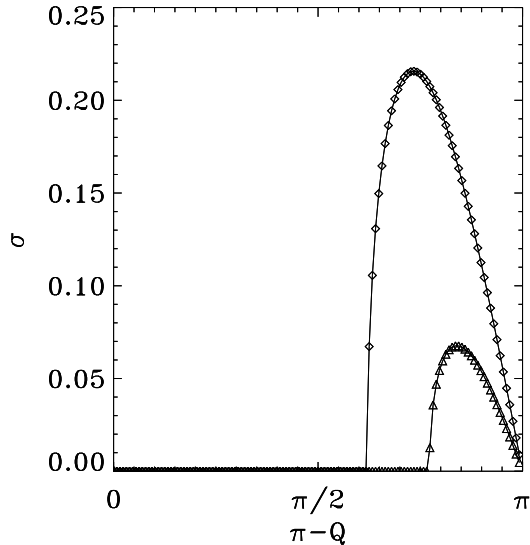


Figure 1: Shape of the growth rate $\sigma(\pi, Q)$. The diamonds correspond to an amplitude $a = 1$ whereas the triangles to $a = 0.5$.

regions in the plane of the parameters $\varepsilon = E/N$ and $\rho(Q) = \cos^2(Q/2)$. In particular, the marginal stability line ε_0 , associated to the vanishing of $\sigma(\pi, Q)$, and the line $\varepsilon_M = \rho(Q_{max})$ are reported. For the marginal stability line ε_0 , our results are fully consistent with a previous theoretical estimation reported in [9].

The above results can be generalized to any power p . In particular, limiting the analysis to the π -mode, the instability condition (9) takes the form

$$\cos^2 \frac{Q}{2} > \frac{1 + \alpha}{1 + (2p + 1)\alpha}, \quad (14)$$

where α is now given by $\alpha = \beta \frac{(2p+1)!}{p!(p+1)!} \left(2\phi_0 \sin \frac{Q}{2}\right)^{2p}$. One can therefore derive the critical amplitude above which the π -mode is unstable and for large N we have

$$a_c \simeq \left[\frac{\pi^2 p!(p+1)!}{2p\beta N^2 (2p+1)!} \right]^{\frac{1}{2p}} \propto N^{-\frac{1}{p}} \quad (15)$$

It means that (for fixed N) a_c is an increasing function of the power of the coupling potential with asymptotic limit $\lim_{p \rightarrow \infty} a_c = 0.5$. Therefore, in the hard potential limit the critical energy density for the π -mode is finite ($\varepsilon_c = 0.5$) for any finite N -value. It should be noticed that this is not in contradiction with the integrability of a one-dimensional system of hard rods, because in the present case we have also a harmonic contribution at small distances.

Finally, we observe that, for the generalized FPU-model, in the high energy limit the growth rate $\sigma_p(\pi, Q) \approx \sqrt{\alpha} \bar{\sigma}_p(\pi, Q)$, where $\bar{\sigma}_p(\pi, Q)$ is independent of the energy. In summary, for high enough values of the energy,

$$\sigma_p(\pi, Q) \propto \varepsilon^{\frac{1}{2} - \frac{1}{2(p+1)}}. \quad (16)$$

We will see in the last section that this scaling law can be also derived from simple dimensional arguments.

Let us now report an analytical estimation of the maximal Lyapunov. As the system is Hamiltonian, Pesin's theorem allows us to identify the Kolmogorov-Sinai entropy S_{KS} with the sum of all positive Lyapunov exponents. As the Lyapunov spectrum was shown [18] to be approximately linear at high

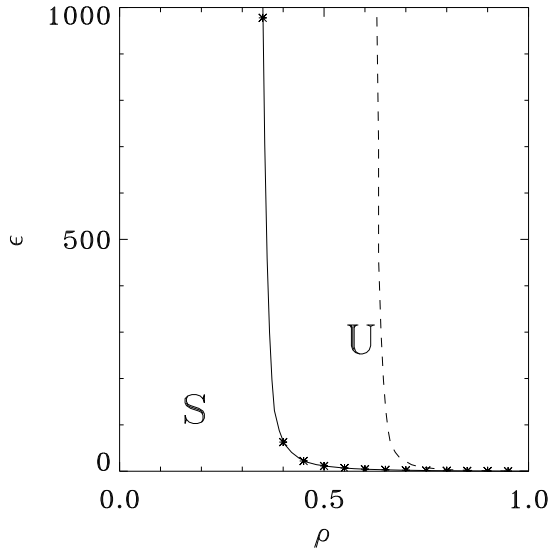


Figure 2: The solid line corresponds to the marginal stability curve ε_0 , the dashed one to $\varepsilon_M = \varepsilon(\rho_{\max})$ and the symbols to the points analytically found by Poggi and Ruffo [9]. The symbols S and U denote stable and unstable region, respectively, separated by the solid line.

energy, one can relate S_{KS} to the maximal Lyapunov exponent λ_1 , namely

$$S_{KS} = \sum_{i=1}^N \lambda_i \cong \lambda_1 \frac{N}{2} \quad . \quad (17)$$

Let us define a new quantity : the instability entropy

$$S_{IE}(q) = \sum_{i=1}^{N/2} \sigma(q, 2\pi i/N) \quad , \quad (18)$$

where the sum is over all positive growth rates [19]. Our crucial physical *ansatz* is that $S_{KS} \simeq S_{IE}(\pi)$. From this assumption the following expression for the maximal Lyapunov exponent is readily derived:

$$\lambda_1 = \frac{2}{N} S_{IE}(\pi) \quad . \quad (19)$$

Employing the analytical values for $\sigma(\pi, Q)$ reported in Eq. (13), λ_1 can be finally computed. Fig. 3 attests that the analytical expression (19) is very accurate. In the same figure the data obtained with a completely different approach, developed by Casetti, Livi and Pettini (CLP) [8], are also shown. The two methods give almost identical results, apart at very low energy, where the CLP findings [8] is in better agreement with our numerical data [10]. In particular, the low energy scaling turns out to be $\lambda_1 \sim \varepsilon^2$, instead our formula gives $\lambda_1 \sim \varepsilon^{1.5}$.

As a matter of fact, we obtain a very good agreement between our theoretical estimation and the numerical results also for $p = 2$ and 3 (see Fig. 3). Plotting $\lambda_1(E/N)$ in a log-log scale we observe (see Fig. 3) that at high energy an asymptotic linear behaviour is found for $p = 1, 2$ and 3 . In the low energy limit, however, for any p the same scaling behaviour should be found, as confirmed by the data reported in Fig. 3. The two asymptotic linear behaviors (at high and low ε) are separated by a knee at intermediate ε . An estimation of this transition value can be obtained 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 [6] which defines the crossing from weak to strong

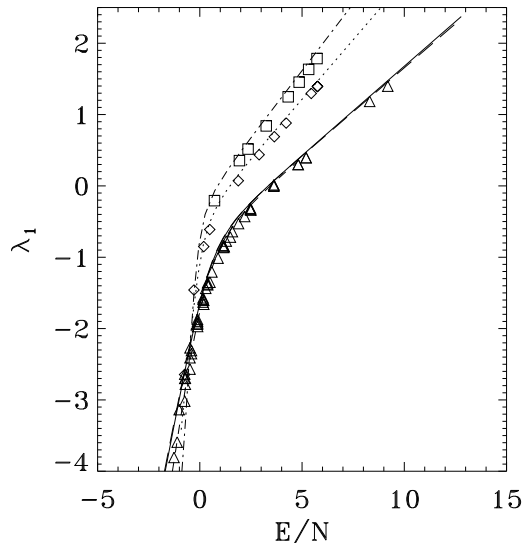


Figure 3: Comparison of the analytical estimate with numerical results for the maximal Lyapunov exponent. The solid curve corresponds to our estimation (Eq. 19), the dashed curve to the CLP-estimate using Riemannian differential geometry (see Ref. [8]) and the triangles to our numerical results (for the β -FPU, i.e. $p = 1$). The dotted curve (resp. diamonds) corresponds to the analytical estimate (resp. numerical results) for $p = 2$ and the dash-dotted (resp. squares) to the analytical estimate (resp. numerical results) for $p = 3$.

chaos and has been called strong stochasticity threshold (SST) (similar SST-transitions have been recently identified also for other models of nonlinear chains [20]). However, we have also found that it corresponds to a crossover from extended to a more localized state in tangent space [10].

It is remarkable to note that Chirikov [21] 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 (13) 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 [22], and although it cannot be used as a signature of chaos, it can give an approximate estimation of λ_1 .

In fact, one can understand this average 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 [9]. The calculation of the instability entropies of this three modes shows that they are extremely close one to another, contrary to the value for other modes. Recently, it has been found that very good estimates for λ_1 can be obtained by applying the CLP method directly to any of the above three one-modes solutions [23]. This confirms that the dynamics of these one-mode solutions is quite peculiar, because they seem to be "optimal" trajectories in the phase-space to estimate the maximal Lyapunov exponent.

The normalized instability entropy $2S_{IE}(q)/N$ is plotted against q and ε in Fig. 4. This should be compared with Fig. 2a in Ref. [24], where a similar plot is reported for the Lyapunov exponent computed from the true Jacobian matrix, but taking the linear Fourier modes as approximate orbits (moreover the case of fixed boundary conditions is considered). At fixed ε both these quantities initially grow with q (low q 's are more stable than high q 's), but then a "stability" region (meaning that the growth rate of the instability is significantly smaller) is present around $q = 2\pi/3$ (numerically estimated as 0.7π by Yoshimura in Ref. [24]). The "ridge" structure observed in [24] reduces in our case to two peaks. The location of the first one depends on ε and reaches $q \approx 0.562\pi$ for large energy density (it is around 0.5π in the region explored by Yoshimura). The second peak is at $(N-2)\pi/N$, and thus goes to π in the $N \rightarrow \infty$ limit. We remark that our evaluation of the instability takes fully

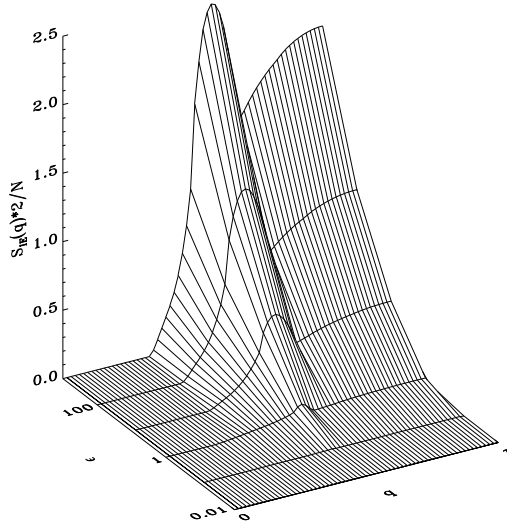


Figure 4: Normalized instability entropy $2S_{IE}/N$ as a function of q and ε .

into account nonlinear effects, contrary to Yoshimura’s, and that it is completely analytical (apart from the necessary numerical evaluation of the roots of Eq. (8)). Mainly, we can confirm that a “stability” region (in the previous sense) is present around $q = 2\pi/3$, which corresponds to one of the exact solutions found in Ref. [9].

4 HIGH ENERGY LIMIT

Here, our claim is that in the high energy limit the temporal evolution of system (1) is essentially ruled by a single time-scale. This time-scale can be easily derived by a simple dimensional argument (see also [7]). At high energy density the potential energy per particle scales as $\frac{V}{N} \sim u^{2p+2}$, where u is the typical size of u_n , and similarly for the kinetic energy per particle $\frac{K}{N} \sim \dot{u}^2$. Assuming a virial of kinetic and potential energies (this is shown to hold for the FPU model in Ref. [25]) $\frac{V}{N} \sim \frac{K}{N} \sim \frac{\varepsilon}{2}$, we can introduce a typical time scale

$$\tau \sim \frac{u}{\dot{u}} \sim \varepsilon^{-\frac{1}{2} + \frac{1}{2(p+1)}} \quad (20)$$

Therefore, the scaling reported in Eq. (16) is easily recovered and it is natural to expect that the same scaling should hold also for λ_1 . In particular, for $p = 1$, λ_1 scales as $\varepsilon^{1/4}$ (as also found in Ref. [8]).

A different scaling, with power $2/3$, was found in Ref. [26] at smaller energy densities (closer to the strong stochasticity threshold (SST), the knee of Fig. 3). A random matrix approximation [27] was invoked to explain these results, which is legitimate only if the process is uncorrelated and one is approaching an integrable limit, where the Lyapunov exponent vanishes. Both these approximations cannot hold exactly in the region where the $2/3$ exponent was found, although a fast decrease of the Lyapunov exponent at the knee could mimic the vanishing exponent situation.

For the β -FPU model ($p = 1$) in the high energy limit, an identical scaling has been recently found by Lepri [28] for the decay-rate of the time autocorrelation functions of the Fourier modes and in Ref. [17] for the inverse of the equipartition time. We have also verified that the normalized Lyapunov spectrum $\tilde{\lambda}_i = \lambda_i/\lambda_1$ converges to an asymptotic shape (independent of ε) for $\varepsilon \rightarrow \infty$. These results confirm our assumption that the dynamics of the system is essentially ruled by an unique time-scale for sufficiently high energy density.

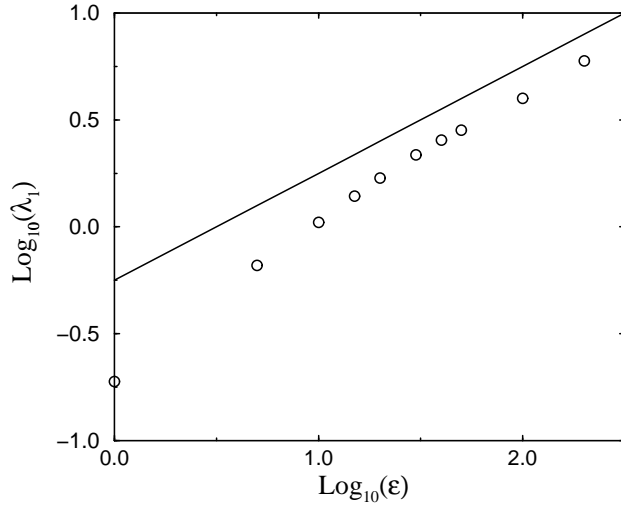


Figure 5: Logarithm of the maximal Lyapunov exponents for the TCL lattice model as a function of the logarithm of the energy density ε . Circles represent our numerical data obtained with $N = 64$ and adopting a 6-th order symplectic integrator [31], with a relative energy conservation ranging from 10^{-12} to 10^{-6} . The solid line refers to a slope 0.5.

It is important to stress that in the limit of hard core potentials ($p \rightarrow \infty$) we find $\lambda_1 \sim \varepsilon^{1/2}$. Moreover, also for potentials that are repulsive (i.e. diverge as $(x - c)^{-q}$ for $x \rightarrow c$ with $q \geq 1$, or even steeper), we argue that the maximal Lyapunov exponent scales as $\varepsilon^{1/2}$ in the high energy density limit. This claim is also supported by the numerical results in Ref [20], where the author studies three different types of potentials, with a repulsive part at short distances: a diatomic Toda lattice, a truncated Coulomb potential (TCL) $V(x) = \frac{1}{2}[\frac{1}{x+1} + x - 1]$ and a Lennard-Jones (LJ) potential. For the TCL potential and the LJ potential, small deviations from the $1/2$ power are found by Yoshimura, but these tend to reduce as the energy density increases, as shown by our simulations of the TCL model reported in Fig. 5. In Ref. [20] also the equipartition times are reported, whose scaling with ε at high energy density is always consistent with an exponent $-1/2$.

Finally, for a gas of hard spheres in a three dimensional box the analogue of the energy density is the temperature T . It is well known that for this model the characteristic time is represented by the Enskog collision time τ_E , which for constant density is proportional to $T^{-1/2}$ [29]. This result suggests that the scaling law $\tau \sim \varepsilon^{-1/2}$ should be valid also for a gas of hard spheres at constant density even in three dimensions, as confirmed by recent data for λ_1 [30].

5 CONCLUSIONS

We have shown that the mechanism of modulational instability of a plane wave (for the three admissible exact one-mode solutions) is strictly connected to Lyapunov instability and its study gives quantitative formula for the maximal Lyapunov exponent. This is still somewhat mysterious, because this mechanism deals with the short-time behavior, while the Lyapunov instability arises from an infinite-time average. One possible explanation of the mystery is that the considered unstable orbits perform a good enough sampling of the phase space, which is uniformly visited by a generic orbit in the equipartition state.

Scaling laws for the Lyapunov exponent at high energy density for generalized FPU chains have been obtained using the modulational instability approach, but it is also observed that they can be easily guessed by simple dimensional arguments. This points to the existence of a universal time scale at high energy, independent of the considered quantity (whether it is the Lyapunov exponent or a correlation function). The same universality holds for hard core potentials.

Acknowledgements

We would like to thank U. Balucani, R. Franzosi, S. Lepri, P. Poggi, A. Politi and A. Rapisarda for enlightening discussions as well as L. Casetti, R. Livi and M. Pettini, for providing us some of their data. T.D. gratefully acknowledges EC for financial support with grant ERBFMBICT961063. This work is also part of the European contract ERBCHRXCT940460 on “Stability and universality in classical mechanics”. S.R. acknowledges the hospitality of the *Centro Internacional de Ciencias* in Cuernavaca, México and the financial support of the same Center and of CONACYT. Part of CPU time has been nicely supplied by the Institute of Scientific Interchanges (ISI) of Torino.

Giovanni Paladin gave important contributions to the theory of Lyapunov exponents, we think he would have been interested in these results.

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