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Normal modes on average for purely stochastic systems

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Abstract

We study a class of non-integrable systems, linear chains with homogeneous attractive potentials and periodic boundary conditions, which are not perturbations of the harmonic chain. In particular, we deal with the system H_4 with a purely quartic potential, which may be shown to be stochastic without any transition. For this model we prove the following pseudo-harmonic properties: (1) the existence of a spectrum of frequencies which are proportional to the harmonic ones, according to a well defined law; (2) the separability on average of the Hamiltonian function among normal modes with these frequencies. Moreover, as far as stochasticity and pseudo-harmonicity are concerned, H_4 is the limit of the Fermi–Past–Ulam (FPU) chain when the energy density tends to infinity. In this frame, the same results as previously obtained for the FPU chain at high energy density are proven to be independent of the presence of the harmonic potential, and to hold at arbitrarily high energies. As a byproduct, we have a stochasticity indicator based on correlations which proves to be very efficient and reliable.

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1. Introduction

The possibility of 'order within chaos' has been widely discussed in the context of dynamical systems, both abstract [1] and classical [2]. For Hamiltonian systems, the coexistence of some kind of order with stochastic features (such as positive Lyapunov exponents, decay of correlations, tendency to equipartition etc) is a topic of argument which periodically reappears, as the complementary problem of possible stochasticity in quasi-integrable systems [3–7].

The prototype model for this kind of study is the Fermi–Pasta–Ulam (FPU) nonlinear chain [8], mostly treated as a perturbation of the harmonic chain. We shall refer in particular to the chain with quartic anharmonicity. Among recent results, we may quote the important phenomenon of 'chaotic breathers', giving rise to localization processes [9]: they appear in a perturbative approach to exact breathers [10], requiring a tight attention to exact solutions corresponding to particular initial conditions.

In the same model, another class of order phenomena regards the spectral properties of time series associated with observables. It has been established [11, 12] that, for the energy density $u = E/N$ even above the so-called 'strong-stochasticity threshold' [4], there exists a pseudo-harmonic spectrum of excitations, for which the harmonic modes work as 'normal modes on average', for generic initial conditions.

Analytical estimates of such a spectrum were presented in [11] but not as a rigorous theorem, so that their excellent confirmation by numerical experiments in [12] was not redundant. However, some problems remain open:

- the harmonic term plays a trivial role and it can even be dropped from the beginning in the analytical estimates but not in the numerical experiments, which have been performed on the complete FPU model, so the influence of the underlying harmonic structure cannot be excluded;
- there exists, in principle, the possibility of a further transition at extremely high energy density, leading FPU to a higher type of stochasticity (for example: the pseudo-harmonic spectrum evolving toward white noise).

Bearing all this in mind, we shall resume the problem of pseudo-harmonicity within the stochastic regime, by studying a model with a purely quartic potential, named in the following H_4, which will be shown to possess the following properties:

- obviously, at no energy can it be looked at as a perturbation of the harmonic chain;
- it is stochastic for all energies;
- it has 'normal modes on average', to the same extent as FPU;
- simple dimensional analysis can be applied, giving further support to the previous difficult estimates in [11];
- its behaviour can also be read, via a rescaling procedure, as the asymptotic energy behaviour of FPU.

From all these points, answers to the problems listed above follow: pseudo-harmonicity does not depend on the harmonic potential, and in FPU there is no further stochastic transition as $u \to \infty$.

Incidentally, for both H_4 and FPU, a simple mechanical origin can be found, i.e. a mass suspended between two identical Hooke springs [13]. If the springs are stretched by a distance d when the mass is in its equilibrium position, both a quadratic and a quartic potential acts on the mass; if the springs are unextended in the same position, only the quartic potential is effective. The transition from a single particle to a chain is obtained by setting the extremities of the springs, connected in couple, on two slides without friction.

2. Notations and models

Consider a chain of N particles of mass m with periodic boundary conditions interacting through confining and translationally invariant potentials U_n:

$$U_n = \lambda_n V_n \qquad V_n = \frac{1}{n}\sum_{i=1}^{N}(x_i - x_{i+1})^n \qquad x_{N+1} = x_1 \tag{1}$$

with $n = 2, 4, 6, \dots$; in the following we shall use $\chi = \lambda_2/2$ and $\varepsilon = \lambda_4/4$, both non-negative, as in previous papers. Clearly, $n = 2$ gives the harmonic potential, and the usual change of variables

$$\begin{vmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{vmatrix} = \boldsymbol{B} \begin{vmatrix} \boldsymbol{x} \\ \dot{\boldsymbol{x}} \end{vmatrix} \tag{2}$$

diagonalizes the Hamiltonian:

$$H_2 = K + \chi\, V_2 = \sum_{k=1}^{N} \left[\frac{1}{2m}\, p_k^2 + \frac{1}{2}\, \omega_k^2 q_k^2 \right] \tag{3}$$

with

$$\omega_k^2 = \chi\, \sigma_k^2 \qquad \sigma_k = 2 \sin \frac{(k-1)\pi}{N} \qquad V_2 = \tfrac{1}{2} \sum_{k=1}^{N} \sigma_k^2 q_k^2. \tag{4}$$

Since the matrix $\boldsymbol{B}$ does not depend on the coupling constant, the same transformation can be performed also on systems with greater n. In particular, the Hamiltonian $H_4(\boldsymbol{q}, \boldsymbol{p})$ reads

$$H_4 = K + \varepsilon\, V_4 = \frac{1}{2m} \sum_{k=1}^{N} p_k^2 + \frac{\varepsilon}{4} \sum_{i=1}^{N} [x_i(\boldsymbol{q}) - x_{i+1}(\boldsymbol{q})]^4 \tag{5}$$

and the FPU Hamiltonian H_{F}, containing both V_2 and V_4, reads

$$H_{\mathrm{F}} = K + \chi\, V_2 + \varepsilon\, V_4 = \frac{1}{2m} \sum_{k=1}^{N} p_k^2 + \frac{1}{2} \sum_{i=1}^{N} \omega_k^2 q_k^2 + \frac{\varepsilon}{4} \sum_{i=1}^{N} [x_i(\boldsymbol{q}) - x_{i+1}(\boldsymbol{q})]^4. \tag{6}$$

The transformation (2) does not diagonalize the potential V_4 and we leave it in implicit form.

For every observable f the time average is defined as usual:

$$\langle f \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T f(\boldsymbol{q}(t), \boldsymbol{p}(t))\, \mathrm{d}t. \tag{7}$$

In the following, time averages will be labelled with an index indicating which Hamiltonian provides the evolution: $\langle f \rangle_4$ and $\langle f \rangle_{\mathrm{F}}$ for H_4 and H_{F}. We refer to [12] for details of the calculations presented below.

3. The FPU model

We recall some properties of FPU, relevant to our purposes. The strong stochasticity threshold can be recognized, e.g., in the crossover of the largest Lyapunov exponent (LLE), described for instance in [14]. This is shown in figure 1 (discussed below).

As for the pseudo-harmonic spectrum, we briefly summarize the procedure in [11]. Consider the formula

$$\langle p_k^2 \rangle_{\mathrm{F}} = \tilde{\omega}_k^2\, \langle q_k^2 \rangle_{\mathrm{F}} \qquad \tilde{\omega}_k^2 = (1 + \alpha_{\mathrm{F}})\, \omega_k^2 = (1 + \alpha_{\mathrm{F}})\, \chi\, \sigma_k^2 \qquad k = 1, \dots, N. \tag{8}$$

Without any further assumption, it represents the definition of α_{F}, which, *a priori*, depends on k. However, from numerical experiments, this quantity appears to be the same for all the modes. This fact is not trivial at all and an analytical estimate of (8) was given, leading to α_{F} actually independent of k:

$$\alpha_{\mathrm{F}} = 2\, \frac{\varepsilon}{\chi}\, A_{\mathrm{F}} \left\langle \frac{V_2}{N} \right\rangle_{\mathrm{F}} \tag{9}$$

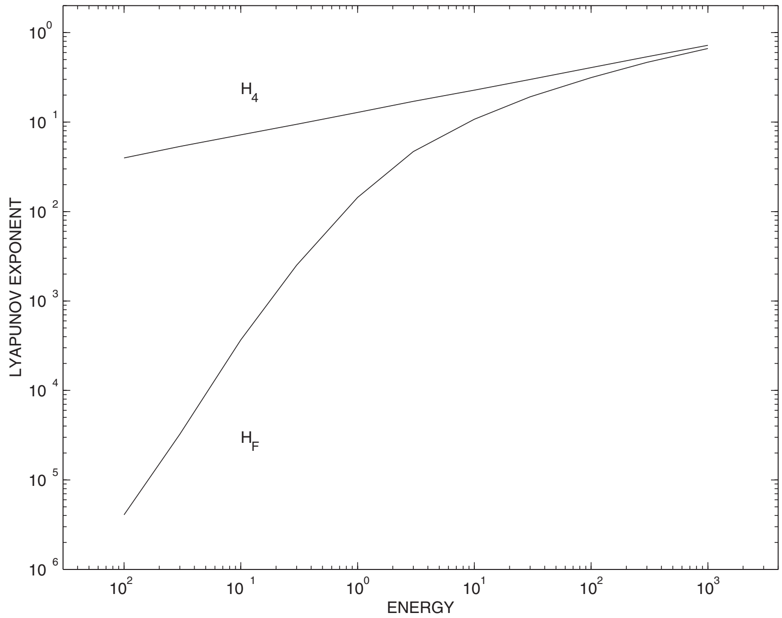

Figure 1. Maximal Lyapunov exponent for H_4, above, and for H_{F}, below, $N = 64$, as functions of energy density u.

where A_{F} is defined as the correlation among time averages of V_2 and V_4:

$$\left\langle \frac{V_4}{N} \right\rangle_{\mathrm{F}} = A_{\mathrm{F}} \left[\left\langle \frac{V_2}{N} \right\rangle_{\mathrm{F}} \right]^2 . \tag{10}$$

$\langle V_2/N \rangle_{\mathrm{F}}$ can be obtained by substituting (8)–(10) in the time average of the energy (6), finally leading to

$$\alpha_{\mathrm{F}} = \frac{2}{3} \left[\left(1 + \frac{3\,\varepsilon\, u\, A_{\mathrm{F}}}{\chi^2} \right)^{1/2} - 1 \right] . \tag{11}$$

Correlation A_{F} has to be determined experimentally, but a few observations are in order. It is a dimensionless parameter, which can depend on $N, m, \varepsilon, \chi, u$, and also on the phase point for u below the stochasticity threshold. Above it, time averages in (10) do not depend on initial conditions (apart from u), and A_{F} does not either. Therefore, above the threshold, it can depend only on N and on the other dimensionless parameter of the system:

$$a = \frac{\varepsilon\, u}{\chi^2} \Longrightarrow A_{\mathrm{F}} = A_{\mathrm{F}}(a, N). \tag{12}$$

Numerical experiments reported in [11] and [12], have shown that:

- actually, the correlation A_{F} does not depend on N, for N sufficiently large, in the whole wide range of the experiments, even below threshold; furthermore, it has finite limits for both $a \to 0$ and ∞;
- frequencies $\tilde{\omega}_k$ are real oscillations of the system as observed in time series of global quantities, e.g. K, even above threshold;
- expression (11) is extremely accurate below and above threshold.

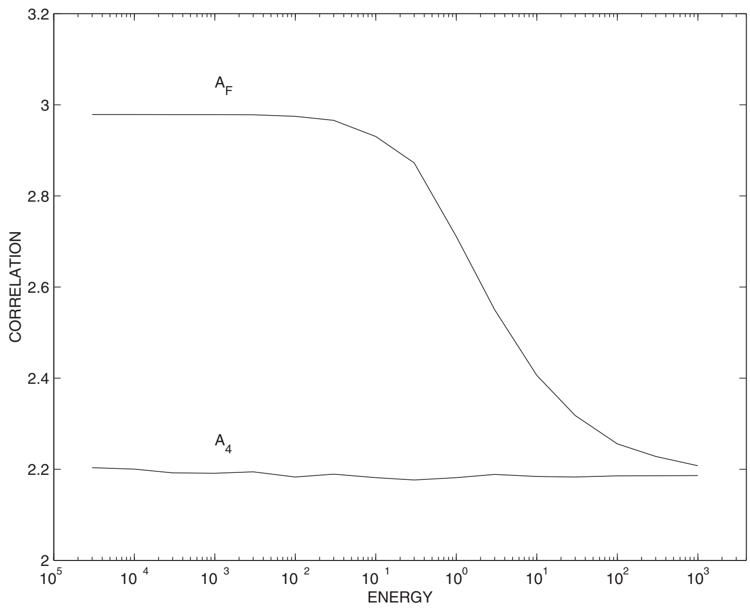

Figure 2. Correlation parameters A_4, below, and A_{F}, above, $N = 64$, as functions of energy density u.

Formula (8) represents a 'generalized virial formula', with the coordinates $(\boldsymbol{q}, \boldsymbol{p})$ playing the role of 'normal modes on average'.

Figures 1 and 2 show that LLE and A_{F} undergo a transition at the same value of the order parameter u. This suggests that A_{F} is very sensitive to the stochastic transition. Furthermore, its stabilization is much faster than for LLE, which requires extremely long averages and a great accuracy in numerical integration. The stability when varying the sampling is very good. Figure 2 is for $N = 64$ and the other cases have not been reported because they are practically identical. The figures contain also the corresponding results for H_4, treated in the following.

Finally, by summing up over k in (8) and taking (9) into account, it follows:

$$\langle K\rangle_{\mathrm{F}} = \chi\,(1+\alpha_{\mathrm{F}})\,\langle V_2\rangle_{\mathrm{F}} = \chi\,\langle V_2\rangle_{\mathrm{F}} + 2\,\varepsilon\langle V_4\rangle = \langle U_2 + 2U_4\rangle_{\mathrm{F}} \tag{13}$$

which appears as a global virial estimate for the inhomogeneous potential of H_{F}.

4. The H_4 chain

The stochasticity of the H_4 model can be tested through the LLE, as described before. The results are given in figure 1, together with those on FPU. These experiments show that H_4 does not undergo any stochastic transition: not only is its exponent always positive, but it has no crossover in the whole range of energy, and it has the same scaling law ($u^{1/4}$) as FPU has when $u \to \infty$.

As for the pseudo-harmonicity of H_4, i.e. the existence of 'normal modes on average', we may proceed in three ways.

(I) All the previous procedure leading to (11) can be resumed just by adapting the proofs in [11] to the purely quartic model H_4. In fact, in formula (8), the addendum 1 trivially takes into account the contribution of the harmonic potential, and this can be omitted from the proofs from the beginning.

(II) In order to avoid tedious comparisons and the heavy estimates of (I), a simpler approach can be applied by exploiting the ordinary virial theorem, valid for H_4 because of its homogeneous potential. Consider the expression similar to (8):

$$\langle p_k^2\rangle_4 = \hat{\omega}_k^2\,\langle q_k^2\rangle_4 \qquad \hat{\omega}_k^2 = \alpha_4\sigma_k^2. \tag{14}$$

For α_4, the independence of k is *assumed here as an ansatz*, disregarding the estimates made in the appendix of [11]. By summing up over k, it follows:

$$\langle K\rangle_4 = \alpha_4\,\langle V_2\rangle_4. \tag{15}$$

This expression reminds us of the virial theorem, which in the actual case reads

$$\langle K\rangle_4 = 2\,\langle U_4\rangle_4 = 2\,\varepsilon\langle V_4\rangle_4. \tag{16}$$

The connection between these two formulae is achieved by the correlation A_4 defined by

$$\left\langle\frac{V_4}{N}\right\rangle_4 = A_4\left[\left\langle\frac{V_2}{N}\right\rangle_4\right]^2. \tag{17}$$

Substituting (17) into (16) and by comparison with (15), we obtain

$$\alpha_4 = 2\,\varepsilon\,A_4\left\langle\frac{V_2}{N}\right\rangle_4. \tag{18}$$

Furthermore, formulae (16) and (17), substituted in the time average of (5), lead to

$$E = \langle H_4\rangle_4 = \langle K\rangle_4 + \varepsilon\,\langle V_4\rangle_4 = 3\,\varepsilon\,A_4\,N\left\langle\frac{V_2}{N}\right\rangle_4^2. \tag{19}$$

Formula (18), with $\langle V_2/N\rangle_4$ derived from (19), finally reads

$$\alpha_4 = 2\sqrt{\frac{u\,\varepsilon\,A_4}{3}}. \tag{20}$$

The dimensionless correlation A_4 must be determined experimentally, as much as A_{F} but in easier conditions: since H_4 is stochastic for all u, A_4 can depend only on m, ε, u and N (see the discussion following (11)). However, since no dimensionless quantity can be formed from m, ε and u, A_4 actually can depend only on N. Figure 2 confirms the independence of u, and experiments not reported here show independence also of N, at least for $N \geqslant 64$.

Note that (17) can be rewritten as

$$\langle V_4\rangle_4 = A_4\left\langle\frac{V_2}{N}\right\rangle_4\frac{1}{2}\sum\sigma_k^2\langle q_k^2\rangle_4 \tag{21}$$

and, using for $\langle V_2/N\rangle_4$ the value obtained from (19), the total energy can now be expressed as

$$E = \sum_{k=1}^{N}\left[\frac{1}{2m}\langle p_k^2\rangle_4 + \frac{1}{4}\hat{\omega}_k^2\,\langle q_k^2\rangle_4\right]. \tag{22}$$

As (8) for FPU, (14) represents a 'generalized virial formula' and, together with formula (22), it suggests that coordinates $(\boldsymbol{q}, \boldsymbol{p})$ play the role of 'normal modes on average' with frequencies $\hat{\omega}_k$.

As said before, this proof is simpler than that outlined in (I), with the drawback that the analytical estimate of (20) is missing. Finally, note that all this procedure could be extended to Hamiltonians H_n as in (1), with $n \geqslant 6$.

(III) The quasi-harmonic spectrum for H_4 can also be obtained directly, by considering the limit $\chi \to 0$ in previous results for FPU. In this limit $H_{\mathrm{F}} \to H_4$ with the harmonic term playing the role of perturbation of the potential V_4: the potential shape is qualitatively stable

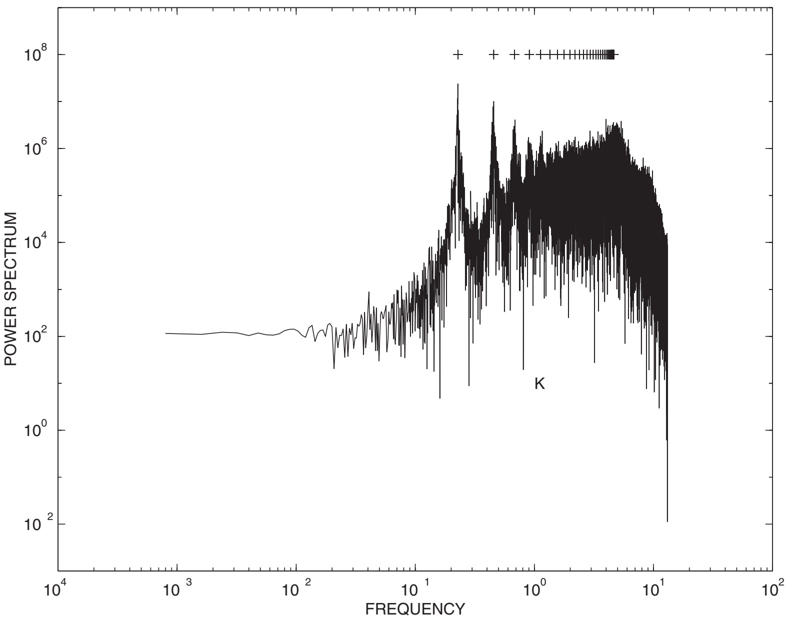

Figure 3. Power spectra at $u = 100$ of kinetic energy K, for the H_4 model, $N = 64$. The + signs mark the frequencies $\hat{\omega}_k$ as given by formula (14) with (20).

and, on physical grounds, we can expect a regular dependence of the solutions at the limit. Note that this is the opposite of the usual perturbative approach with $\varepsilon \to 0$.

Through a direct inspection, formulae (8), (10) and (11) for FPU go to the corresponding (14), (17) and (20) for H_4. More explicitly, for $\chi \to 0$

$$A_{\mathrm{F}} \to A_4 \qquad \chi\, \alpha_{\mathrm{F}} \to \alpha_4 \qquad \tilde{\omega}_k^2 \to \hat{\omega}_k^2. \tag{23}$$

Furthermore, from (13) the virial theorem (16) is obtained.

5. Asymptotic behaviour and conclusions

Generally speaking, the infinite limits cannot be checked experimentally but, in our case, $u \to \infty$ can be shown to be somehow equivalent to $\chi^2 \to 0$. This leads to the possibility of studying the asymptotic energy limit of FPU, through a rescaling of the H_4 results at a finite $\bar{u}$. Consider indeed formula (12): since A_{F}, apart from N, depends only on $a = \varepsilon\, u/\chi^2$, the limits $\chi^2 \to 0$ and $u \to \infty$ are equivalent to each other, and both to $a \to \infty$. Therefore, $A_{\mathrm{F}} \to A_4$ also for $u \to \infty$. As a consequence, from (11), we obtain

$$\chi\, \alpha_{\mathrm{F}} \approx 2\sqrt{\frac{u\, \varepsilon\, A_4}{3}} = \alpha_4 \Longrightarrow \tilde{\omega}_k \approx \hat{\omega}_k \tag{24}$$

for both $\chi \ll 1$ and $u \gg 1$. The real content of (24) is that, since A_4 does not depend on the energy, the asymptotic terms depend on u only through the factor $\sqrt{u}$. Therefore, by rescaling the H_4 pseudo-harmonic spectrum at energy density $\bar{u}$ with $\sqrt{u/\bar{u}}$, results at every high energy u can be obtained for both FPU and H_4.

In order to check the effective existence of frequencies $\hat{\omega}_k$, we have considered a number of observables (kinetic or potential energies, microcanonical density, and other quantities already studied in [12]), and their instantaneous values along the trajectory. The time series, analysed by fast Fourier transform, give power spectra such as in figure 3. The peaks in the figure correspond to the set of frequencies analytically given in (14) with (20), and this is true in the whole range of energy where experiments have been carried out. For the tail of frequencies above the maximal $\hat{\omega}_k$, see discussions in [12] where analogous spectra for FPU were studied. In conclusion, our claims are confirmed by numerical checks: there exists for H_4 a frequency spectrum proportional to the harmonic one, even if there is no harmonic potential in the Hamiltonian. Moreover, H_4 describes accurately the asymptotic behaviour of FPU.

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