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QUASI NORMAL MODES IN STOCHASTIC DOMAINS

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Abstract. In anharmonic chains with even potentials, including classical Fermi-Pasta-Ulam model, we show how ordered structures can coexist with high degree stochasticity.

1. **Introduction.** Since the pioneering work of Fermi, Pasta and Ulam (FPU), anharmonic chains have been the privileged models to explore existence, onset and physical relevance of ergodic properties in classical statistical physics [1], [2].

Investigations in this field insist very often on the connection between non-ergodicity (or order) and KAM theory [2], [3]. In these approaches (classical perturbation theory), the assumption is that only residual invariant surfaces with positive measure can be responsible for lack of ergodicity, with related items as difficulty in reaching equipartition and existence of quasi harmonic modes. The rich variety of behaviours emerging from numerical simulations and contrasting the crude order-desorder dichotomy, has been consequently ascribed to exponential delay in approaching equilibrium, for instance along the lines of Nekhoroshev theorem [4].

We present here some arguments showing that there exist many important statistical and dynamical properties of anharmonic chains which can be explained in different and simpler terms. Precisely:

1) quasi harmonic spectra exist even at high energies, where KAM theory does not apply; they can be detected in finite time experiments, and their asymptotic properties (total energy or number of degrees of freedom going to infinity) can be understood without the intricacies of the thermodynamic limit in classical perturbation theory;

2) there is no contradiction between equipartition and existence of quasi harmonic modes: on the contrary, all the experimental phenomenology about equipartition can be effectively recovered in this frame.

Note that these concepts have to be consistently rephrased. While they are almost obvious in a perturbative context (i.e. for near integrable systems), they could be physically meaningless in the stochastic region. We shall show in which sense harmonic modes keep their meaning and relevance in chains above the so called strong stochasticity threshold (see [5]), or even for intrinsically stochastic chains without the quadratic part [6], [7], [8]. Sometimes, in order to distinguish these modes from those emerging in the perturbative approach, we shall speak of *pseudo* harmonic modes or spectra.

Simple dimensional analysis, an extension of the virial theorem and properties of correlations are sufficient tools to get the results. They are corroborated by previous

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analysis and experimental works [9], based on suitable observables and peculiar phenomena we studied in this context (Frenet-Serret curvatures, rates of energy exchanges and freezing conditions for normal modes). We stress that our results are generic with respect to initial conditions; this means, for instance, that numerical experiments supporting them do not require single or few modes excitations. Moreover, they completely confirm, in terms of correlations, the existence of the strong stochasticity threshold. The thermodynamic limit of this threshold can be understood more easily here than in other approaches.

Finally, our results offer some arguments to distinguish the stochasticity of this class of anharmonic chains from the stochasticity of the hard spheres.

2. **Hamiltonians, Virial Theorem and Equipartition.** Consider a chain of N particles of mass $\mu = 1$ interacting via a sum of translationally invariant potentials U_n of even degree n, with periodic boundary conditions:

$$U_n = \lambda_n \, V_n \quad , \qquad V_n = \frac{1}{n} \sum_{i=1}^{N} (x_i - x_{i+1})^n \ , \ x_{N+1} = x_1 \ , \ n = 2, 4, 6, ... \tag{1}$$

The case of the single potential with $n = 2$ corresponds to the integrable harmonic chain and, by the usual change of variables

$$\begin{vmatrix} \mathbf{q} \\ \mathbf{p} \end{vmatrix} = \mathbf{\Omega} \begin{vmatrix} \mathbf{x} \\ \dot{\mathbf{x}} \end{vmatrix} \ , \tag{2}$$

the system diagonalizes, leading to the Hamiltonian

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

where $\chi \equiv \lambda_2$, and the frequencies are

$$\omega_k = 2\sqrt{\chi} \sin \frac{(k-1)\pi}{N} \ . \tag{4}$$

Since the matrix $\mathbf{\Omega}$ does not depend on the coupling constant χ , the same transformation can be performed also on higher degree potentials, which clearly do not diagonalize. We consider two classical examples, FPU with 2nd and 4th degree interactions

$$H_{\scriptscriptstyle F} = K + \chi \, V_2 + \varepsilon \, V_4 \ = K + \chi \, V_2 + \frac{\varepsilon}{4} \sum_{i=1}^{N} [x_i(\mathbf{q}) - x_{i+1}(\mathbf{q})]^4 \ , \tag{5}$$

and the purely anharmonic quartic model

$$H_4 = K + \varepsilon \, V_4 \ = K + \frac{\varepsilon}{4} \sum_{i=1}^{N} [x_i(\mathbf{q}) - x_{i+1}(\mathbf{q})]^4 \ , \tag{6}$$

where $\varepsilon \equiv \lambda_4$.

Once introduced the Hamiltonian, we can evaluate the usual time average of every observable f along the trajectory:

$$\langle f \rangle_{\scriptscriptstyle T} = \tfrac{1}{T} \int_0^T f(\mathbf{q}(t), \mathbf{p}(t)) \, dt \ , \ \langle f \rangle = \lim_{T \to \infty} \langle f \rangle_{\scriptscriptstyle T} \ . \tag{7}$$

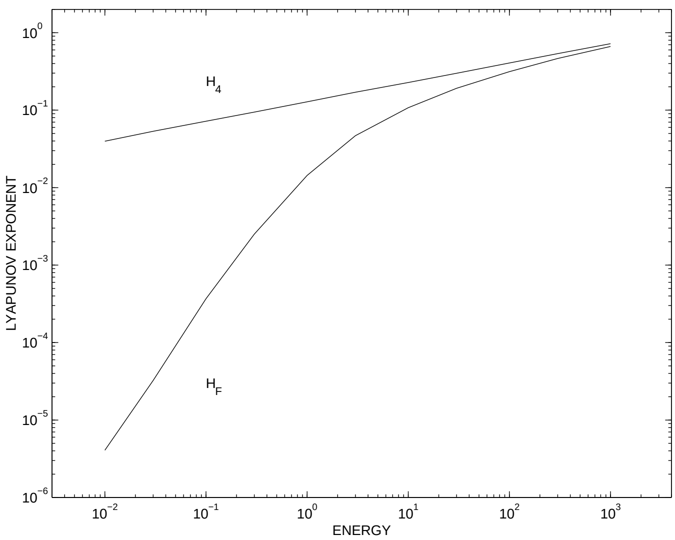

FIGURE 1. Maximal Lyapunov exponent for H_4 and H_F, as functions of specific energy u. Here $N = 64$. See [8].

Finally, as main tools in the following analysis, we remind that, for confining potentials as in (1), the virial theorem holds [6]:

$$\left\langle p_k \frac{\partial H}{\partial p_k} \right\rangle = \left\langle q_k \frac{\partial H}{\partial q_k} \right\rangle , \tag{8}$$

and that, according to equipartition theorem, quantities (8) do not depend on k (see [10]).

3. **FPU Model.** For this model, the virial theorem reads:

$$\langle p_k^2 \rangle_F = \omega_k^2 \langle q_k^2 \rangle_F + \left\langle q_k \frac{\partial U_4}{\partial q_k} \right\rangle_F , \tag{9}$$

where the second term of right hand side contains the anharmonic force on the k-th collective oscillator. Note the index F, to remind explicitly that the time evolution depends on H_F. By summing over k in (9), and by observing that:

$$\sum_k q_k \frac{\partial U_4}{\partial q_k} = \sum_i x_i \frac{\partial U_4}{\partial x_i} = 4 \ \varepsilon \ V_4 , \tag{10}$$

we may write the virial theorem for FPU in the more usual global version:

$$\langle K \rangle_F = \chi \ \langle V_2 \rangle_F + 2 \ \varepsilon \ \langle V_4 \rangle_F . \tag{11}$$

3.1. **The Quasi Harmonicity Ansatz.** Going back to (9), note that the equipartition theorem regards the whole right hand side, not only the harmonic term $\omega_k^2 \langle \ q_k^2 \ \rangle_F$. On the other hand, we cannot neglect the anharmonic potential, since the theorem applies precisely where U_4 is relevant. Therefore, the fact that, experimentally, the harmonic energies $\frac{1}{2}\left[\langle p_k^2 \rangle_F + \omega_k^2 \langle q_k^2 \rangle_F\right]$ undergo equipartition above the strong stochasticity threshold, can be explained by supposing the anharmonic

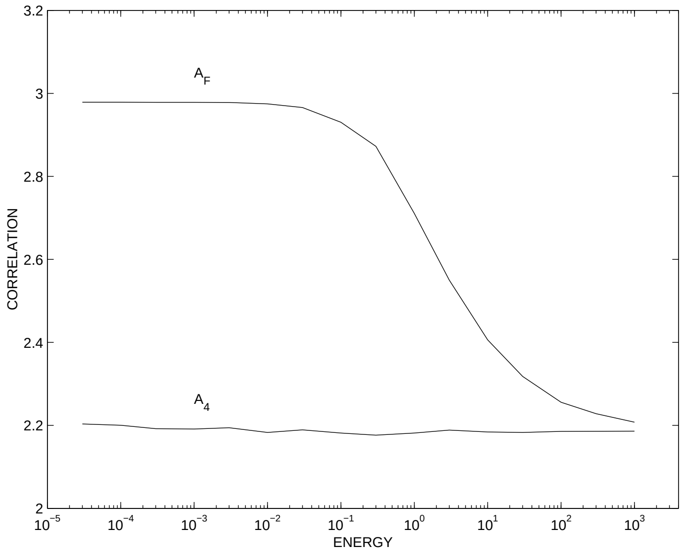

FIGURE 2. Correlation parameters A_4 , and A_F , as functions of specific energy u . Here $N = 64$. See [8].

term to be proportional to the harmonic one. This hypothesis can be expressed in the following way:

$$\langle p_k^2 \rangle_F = \, _F\Omega_k^2 \, \langle q_k^2 \rangle_F \ , \ \ _F\Omega_k^2 = (1 + \alpha_F) \, \omega_k^2 \ , \tag{12}$$

with α_F dependent on the parameters of the model but independent of k . This ansatz has been checked numerically at every sensible value of the parameters, say the specific energy u , below, within and above the stochasticity threshold [6]. In particular, when $u \to 0$ we have $\alpha_F \to 0$ and, as obvious in the perturbative regime, $_F\Omega_k \to \omega_k$. Above threshold, a value of α_F essentially independent of k is reached in a time T much shorter than the equipartition time; moreover, since formula (12) is valid also at very high energy, in this region the pseudo harmonic frequencies $_F\Omega_k$ cannot have a perturbative origin.

3.2. **Correlations.** To study the dependence of α_F on the parameters, we start by summing up the ansatz (12) over k :

$$\langle K \rangle_F = (1 + \alpha_F) \ \chi \ \langle V_2 \rangle_F \ . \tag{13}$$

Then we introduce the correlation parameter A_F between the harmonic and anharmonic potentials:

$$\left\langle \frac{V_4}{N} \right\rangle_F = A_F \ \left[\left\langle \frac{V_2}{N} \right\rangle_F \right]^2 \ , \tag{14}$$

through which the virial theorem (11) can be rewritten as

$$\langle K \rangle_F = \chi \ \langle V_2 \rangle_F + \frac{2 \ \varepsilon \ A_F}{N} \ \left[\langle V_2 \rangle_F \right]^2 \ . \tag{15}$$

By comparing this expression with (13), α_F can be expressed as a function of $\langle V_2 \rangle_F$ only. Then, we substitute the kinetic energy (15) and the anharmonic contribution

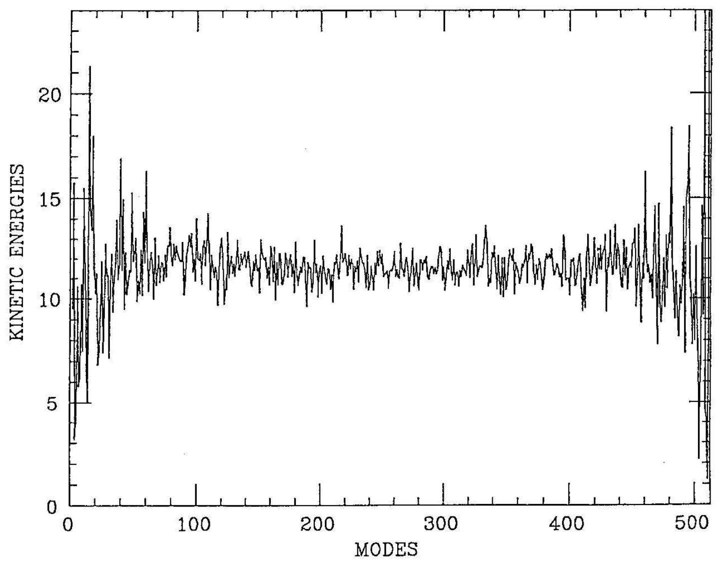

FIGURE 3. Time-averaged kinetic energies $\langle p_k^2 \rangle_F$ evaluated at a finite time T . Parameters: $N = 512$, $u = 10$. See [6].

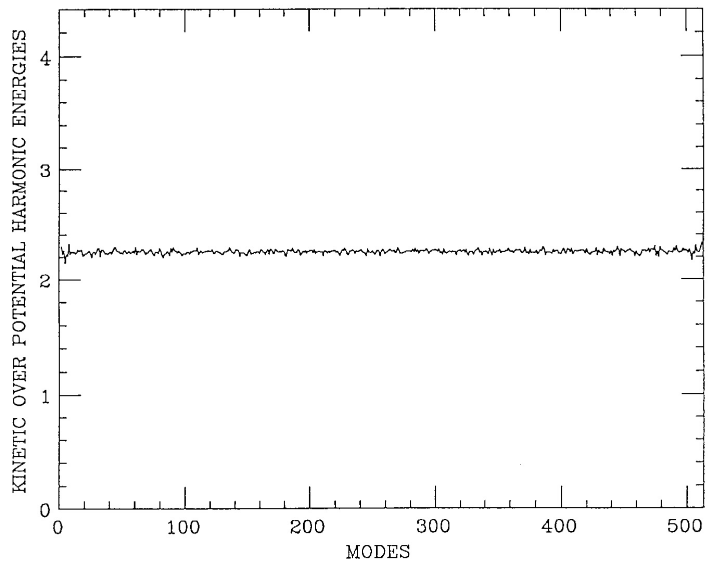

FIGURE 4. Ratio between time-averaged kinetic and potential harmonic energies $\langle p_k^2 \rangle_F / \langle \omega_k^2 q_k^2 \rangle_F$. Same parameters as in Fig.3. See [6].

from (14) in the time averaged Hamiltonian (5) divided by N ; from here, we obtain $\langle V_2 \rangle_F$ which, substituted in the expression of α_F , finally gives:

$$\alpha_F = \frac{2}{3} \left[\left(1 + \frac{3 \, \varepsilon \, u \, A_F}{\chi^2} \right)^{1/2} - 1 \right] \ , \ u = E/N \ . \tag{16}$$

It depends on the parameters of the Hamiltonian, on the initial energy, and on the unknown correlation A_F , which has to be evaluated experimentally.
Formula (12), assumed here as an ansatz, and formula (16), have been analitically derived in [6], by direct but cumbersome estimates.

3.3. **Dimensional Analysis.** A_F is a dimensionless quantity, possibly depending on N and on the unique dimensionless combination of the other parameters, i.e.:

$$A_F = A_F(N, \varepsilon u/\chi^2) \ . \tag{17}$$

Actually, explicit dependences on N have been already introduced in (14) and by the specific energy u , and it seems reasonable that no further dependence survives in (17). This fact has been confirmed by our experiments in the range $N = 32, ..., 1024$, so that A_F can be studied as a function of the specific energy only. We may expect two extreme behaviors, at low and high energy, in correspondence to high and low value of correlation. Therefore, FPU should undergo a transition, with A_F as indicator and the specific energy as order parameter. This is confirmed by experiments, and A_F proves to be very efficient with respect to Lyapunov and equipartition based indicators.

4. **Purely Anharmonic H_4 Model.** As already observed, the transformation (2), which diagonalizes the harmonic Hamiltonian, does not depend on χ and it can be applied even to a Hamiltonian, like H_4 , which does not contain the harmonic potential at all. From here, we could proceed with the same method applied in previous section. More simply, we study the FPU results in the limit $\chi \to 0$, which clearly leads from H_F to H_4 . We obtain:

$$A_F \to A_4 = \frac{\langle V_4 \rangle_4}{\left[\langle V_2 \rangle_4 \right]^2} \ , \ \chi \alpha_F \to \alpha_4 = 2 \sqrt{\frac{u \varepsilon A_4}{3}} \ , \ {}_F\Omega_k^2 \to \ {}_4\Omega_k^2 = \alpha_4 \, \omega_k^2 \tag{18}$$

Since the only relevant parameter both in (16) and in (17) is $\varepsilon u/\chi^2$, the limit $\chi \to 0$ is equivalent to $u \to \infty$, i.e. H_4 is the limit of H_F at infinite energy.
Once again, the relevant point is that α_4 does not depend on index k . What's new in H_4 , with respect to H_F , is that, since one parameter (χ) is missing, the dimensionless A_4 can depend only on N . Actually, we found that A_4 is a constant, and it can be evaluated with a single numerical experiment. In particular, it does not depend on the specific energy u , and we do not expect any transition. H_4 is always stochastic, as the limit of FPU at infinite energy. The same conclusion can be obtained from other indicators, even dimensional ones. In particular, the Lyapunov exponent λ , dimensionally an inverse time, is expressed by:

$$\lambda = c \left(\frac{u\varepsilon}{m^2} \right)^{1/4} ,$$

with c adimensional constant. The scaling law $u^{1/4}$, in the whole range of energy, is easily readable in Fig.1, without any mark of transition.

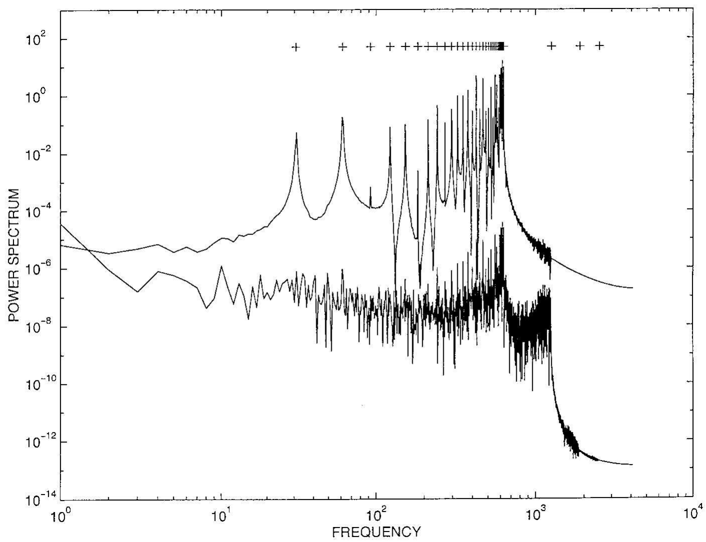

FIGURE 5. Power Spectra at $u = 0.01$ of kinetic energy (above) for FPU, $N = 64$. The $+$ signs mark the frequencies ${}_F\Omega_k$ according to formulas (12) and (16), and A_F from Fig.2. Below, microcanonical density is displayed. See [7].

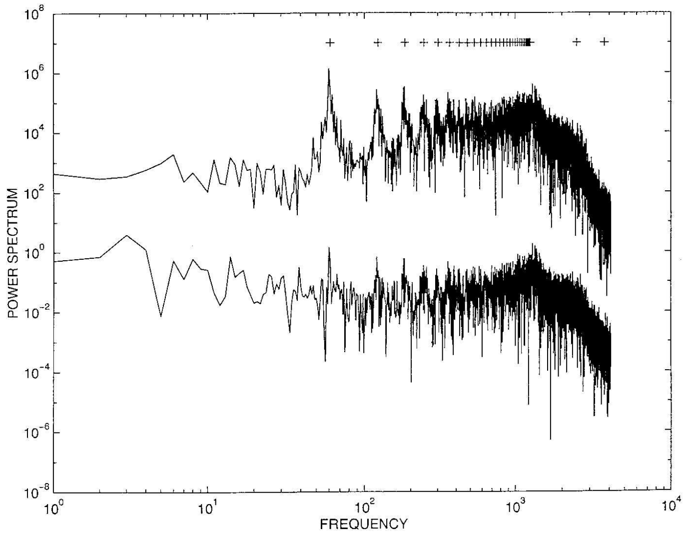

FIGURE 6. Power Spectra at $u = 40$ of harmonic energy (above), for FPU. Parameters and $+$ signs as in Fig.5. Below, microcanonical density is displayed. See [7].

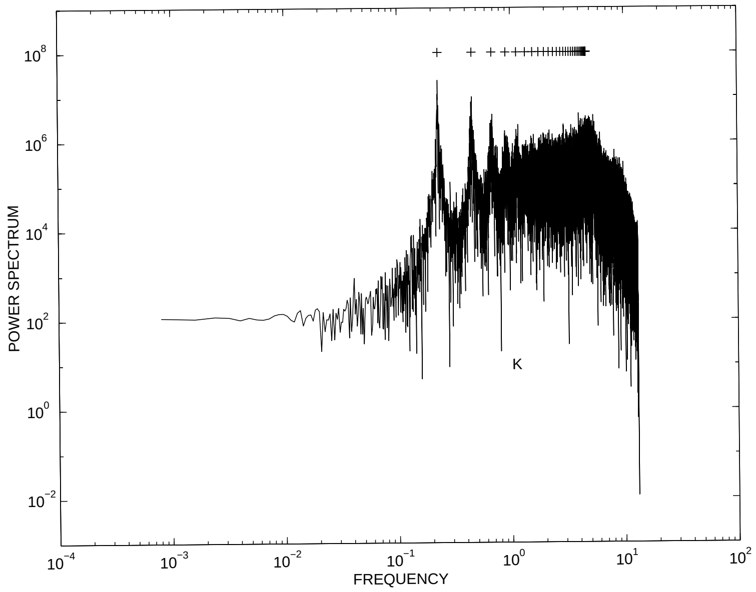

FIGURE 7. Power Spectra at $u = 100$ of kinetic energy for H_4 model, $N = 64$. The $+$ signs mark the frequencies ${}_4\Omega_k$ as given by formula (18), with A_4 from Fig.2. See [8].

5. **Experiments and Conclusions.** To be consistent with standard literature, all our calculations have been performed with $\varepsilon = 0.1$ and $\chi = 1$ or $\chi = 0$ for FPU or H_4. For both systems, consider first the behavior in specific energy of two indicators, the classical maximal Lyapunov exponent, Fig.1, and the correlations A_F and A_4 , Fig.2. The two indicators confirm that H_4 does not undergo any transition, and that FPU has a crossover region between two limit behaviors, at low and high energy, at $u \approx 1$, the strong stochasticity threshold. Furthermore, the two figures show H_4 to be the high energy limit of FPU.

The ansatz (12) for FPU has been checked directly in [6] for all energies. An example of the results above threshold is reported in Fig.3 and Fig.4. Simulations show that α_F attains a good independence of k in a time T much shorter than the equipartition time. At this value of T , kinetic energies $\langle p_k^2 \rangle_F$ are indeed not equipartitioned at all, in particular the low frequencies ones, Fig.3. Implications of this phenomenon on the thermodinamic limit have been discussed in [6].

With the correlations from Fig.2, we also checked the dependence of α_F and α_4 on the parameters, including N (see [6] and [7],[8]).

The last important question to address is the role of quasi (or pseudo) harmonic frequencies ${}_F\Omega_k^2$ and ${}_4\Omega_k^2$. Are they real oscillation frequencies of the variables p_k and q_k , and of meaningful phase observables?

We gave a positive answer already in [6], and a more exhaustive one in [7], Fig.5 and Fig.6, for FPU below and above treshold, and in [8], Fig.7, for H_4 . In these figures, power spectra of harmonic energy, kinetic energy, and microcanonical density are shown, together with ${}_F\Omega_k$ and ${}_4\Omega_k$.

In the case of FPU we added the microcanonical density $\rho = 1/|\nabla H(\mathbf{q}, \mathbf{p})|$, as an instructive example of nonlinear dependence on the $\{p_k^2\}$ and $\{q_k^2\}$. In principle, it could be insensitive of the pseudo harmonic frequencies but, actually, at high energy the whole spectrum is clearly detectable, even if at low energy only the maximal frequency appears.

We can conclude that stochasticity can coexist with ordered structures. Therefore, the type of chaos of anharmonic chains has to be distinguished from the reference idea of chaoticity of the Boltzmann gas. Physical implications of this fact are research matter, for instance in thermal conductivity [11], or in localization processes connected to chaotic breathers [12].

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