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NUMERICAL EXPERIMENTS ON THE STATISTICAL BEHAVIOUR OF DYNAMICAL SYSTEMS WITH A FEW DEGREES OF FREEDOM *

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Numerical experiments concerning the arising statistical laws in a system of nonlinear interacting waves are described. A chain of particles coupled by nonlinear springs has been used as a model. Various statistical properties of the chain have been investigated numerically. A comparison with the theory of the Korteweg–de Vries equation is given.

One of the most interesting problems which has occupied the minds of scientists over a century is the problem of the arising statistical laws in a dynamical system. Now it is firmly established that one does not need for this a large, much less an infinite number degrees of freedom as had been assumed till recently. On the contrary, even the simplest dynamical systems are governed, under certain conditions, by statistical laws. To be more nearly correct, the motion of such systems possesses ergodicity, mixing and positive KS entropy (Krylov–Kolmogorov–Sinai dynamical entropy [1–3]). The latter characterises exponential relaxation of a system to some statistical equilibruim (section 3). We will call this type of motion the stochastic one. Sinai proved rigorously [4] the stochasticity of plane motion of a disk bouncing from an everywhere convex (more precisely, nonconcave) closed curve. This autonomous system has two degrees of freedom only. For the non-autonomous system even one degree of freedom is sufficient. The vibrations of a one-dimensional nonlinear oscillator suffering periodic perturbation can be taken as an example. Contemporary ergodic theory fails to solve this at a first glance simple problem. So, for its investigation one has to fall back upon numerical experiment guided by semiqualitative theory [7]. To the best of our knowledge the first such experiments were carried out by Goward and Hine [5]. Later on this problem has been studied in detail numerically with a model nonlinear transformation $\varphi, \psi \to \bar{\varphi}, \bar{\psi}$ [6–8]:

$$\bar{\varphi} = \{\varphi + \lambda f(\psi)\}\,; \quad \bar{\psi} = \{\psi + \bar{\varphi}\}\,. \tag{1.1}$$

Here φ, ψ stand for canonically conjugated variables simulating the oscillator's momentum and coordinate, respectively; the brackets signify fractional part; λ is a parameter. Even this at a first glance elementary transformation turns out to be beyond the power of today ergodic theory if $f(\psi)$ has a continuous derivative $f'(\psi)$. Stochasticity conditions or, as we shall say, the border of stochasticity for (1.1) has the form:

$$|\lambda f'(\psi)| \gtrsim 4. \tag{1.2}$$

Numerical and analytical studies of stochasticity in simple dynamical systems were done at about the same time by a number of groups in various countries. For reviews of those works and references see, for instance, refs. [7, 9–12].

Below we will describe some numerical experiments with a more interesting model used earlier by Fermi et al. [13].

2. Fermi–Pasta–Ulam (FPU) model

This model was applied in ref. [13] just to clarify the question of statistical relaxation in a non-lin-

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ear system. The model is a chain of identical particles coupled by identical nonlinear springs. The equations of motion are:

$$m\ddot{x}_n = f(x_{n+1} - 2x_n + x_{n-1}) + \beta[(x_{n+1} - x_n)^3 - (x_n - x_{n-1})^3], \quad n = 0, 1, ..., N-1, \tag{2.1}$$

where x_n stands for the deviation from equilibrium of the nth particle; m the particle mass; f the elasticity factor; and β is the nonlinearity parameter. We shall assume henceforth: $m = f = 1$.

The set of equations was integrated numerically for two kinds of boundary conditions: (1) zero boundary conditions (ZBC): $x_0 = x_N = 0$;

(2) periodic boundary conditions (PBC): $x_0 = x_N$.

Obtained data were processed, mainly, in terms of the normal modes of a linear chain ($\beta = 0$). Initial conditions usually had the form of a superposition of several modes.

For numerical experiments to be efficient the choice of a model is perhaps the most important factor. On one hand, it has to be rather simple since the possibilities of todays computers are still very restricted; on the other hand, the model should be interesting enough (nontrivial) for physics. In this respect the FPU model proved to be very successful since it allows one to trace the transition from more or less known discrete nonlinear systems to the nonlinear waves which study is just at the outset.

In particular, for sufficiently large N the set (2.1) corresponds approximately to the nonlinear wave equation [14]:

$$\frac{\partial^2 x}{\partial t^2} = \frac{\partial^2 x}{\partial z^2}\left[1 + 3\beta\left(\frac{\partial x}{\partial z}\right)^2\right] + \gamma^2 \frac{\partial^4 x}{\partial z^4}, \tag{2.2}$$

where $z = na$ is the coordinate along the chain (with step a); $\gamma^2 = a^2/12 = L^2/12N^2$. The accuracy of this approximation is characterized by two small parameters:

$$\alpha \approx \left(\frac{ak}{L}\right)^2; \quad \epsilon \approx 3\beta u^2 \approx 3\beta w, \tag{2.3}$$

where $u = \partial x/\partial z$; $w = E/L$ stands for the density of the oscillation energy; k is the serial number of the mode.

A purely progressive wave is described approximately (to accuracy $\approx \epsilon$) by the first order equation [15]:

$$\frac{\partial u}{\partial \tau} + u^2 \frac{\partial u}{\partial z} + \delta^2 \frac{\partial^3 u}{\partial z^3} = 0; \quad \delta^2 = \frac{2\gamma^2}{3\beta}; \quad \tau = \tfrac{3}{2}\beta(t - z). \tag{2.4}$$

This is generalized Korteweg–de Vries equation (KdV) the solutions of which are notable for their remarkable stability (see section 4).

3. Stochastic motion of a dynamical system

The first experiments with a nonlinear chain [13] revealed no statistical relaxation ($N = 32$). Instead of the expected irreversible equipartition of energy among all the modes, quasiperiodical oscillations of the first few modes were observed. In this connection the authors of ref. [13] have put forward a hypothesis on the existence of some stable nonlinear modes of oscillation. About the same time Kolmogorov proved his famous theorem on the retaining stability of nonlinear oscillations under small perturbation [16]. On the other hand, the nonlinear system with many degrees of freedom must at last relax, under some conditions, to the statistical equilibrium as is required by statistical mechanics.

To resolve this paradox the hypothesis was put forward in ref. [17] that there is a border of stochasticity for the nonlinear chain which divides the system's phase space, roughly speaking, in two parts: stochastic and stable ones. Using the criterion of stochasticity by overlapping nonlinear resonances [18, 7] an analytical estimate was obtained in [17] for the border of stochasticity of a chain ($k \ll N$):

$$\epsilon_s \approx 2m^{1/2}/k, \tag{3.1}$$

where m stands for the number of excited modes, and k is their mean serial number. The surprising results of the work in ref. [13] do not contradict with the criterion (3.1) since lower modes ($k \approx 1$) were usually excited in ref. [13].

The statistical properties of a nonlinear chain were studied in detail in refs. [19, 20] by means of numerical experiments. Below, a brief summary of the main results is given.

The position of the stochasticity border was determined by means of local instability of motion. The

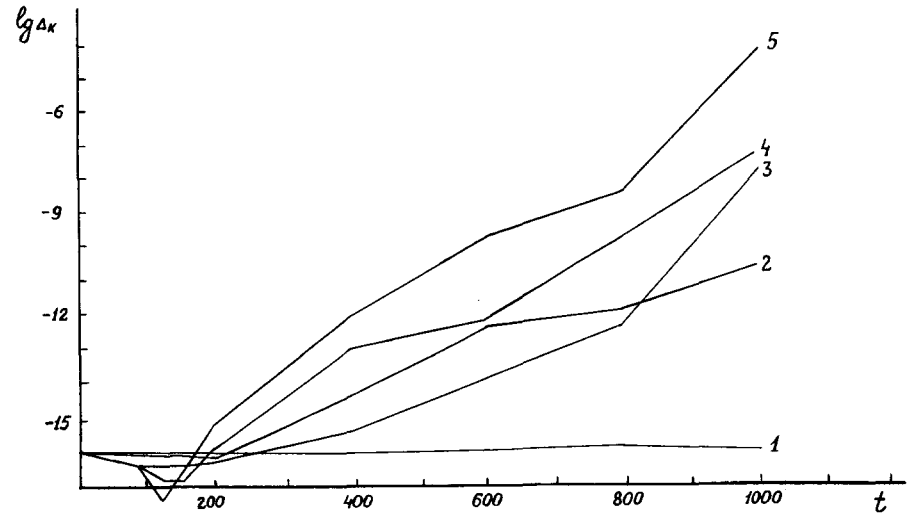

Fig. 1. An example of the local instability of motion in the stochastic region: $\beta = 0.5$ (1); 1.75 (2); 2.0 (3); 2.25 (4); 2.5 (5); $\beta_s = 0.5 \pm 0.1$; Δ_k is a distance between two close trajectories.

latter means that initially close trajectories diverge, on the average, exponentially with time (see fig. 1): $\Delta = \Delta_0 \exp(-ht)$, where Δ is some distance between trajectories. The averaged value of h is just the KS entropy. According to modern ergodic theory [9] this exponential instability leads to mixing and other statistical properties of motion.

The simpliest theory for the nonlinear chain [21, 7] gives (for E = const):

$$h \approx (\Omega/\pi)\ln(\beta/\beta_s) \approx (1/N)\ln(\beta/\beta_s), \qquad (3.2)$$

where β_s relates to the border of stochasticity, and Ω is the lowest frequency of the chain. The experimental dependence $h(\beta)$ is shown in fig. 2.

Comparison of experimental data with the analytical estimate (3.1) for ZBC is presented in table 1. Here k_0 stands for the serial numbers of the initially excited modes. In the analytical treatment the decay of the initial state into solitons (section 4) has been taken into account; this has led to an increase of the mean serial number of the modes: $k_0 \to k \approx \epsilon^{1/2}N$.

Satisfactory agreement is generally observed between the analytical estimates of (3.1) and (3.2) and experiment. The three cases marked with asterisks in table 1 are exceptions. Cases 2 and 3 can be explained qualitatively due to the inapplicability of criterion (3.1) to higher modes. Yet, in case 9 just the opposite effect is observed. The cause of the latter is unknown so far.

In the stochasticity region ($\epsilon \gg \epsilon_s$) the following statistical properties of the chain were observed.

(i) Energy equipartition among the oscillation modes (fig. 3). The decline of the spectrum for lower modes (curve 3) can be explained by the fact that

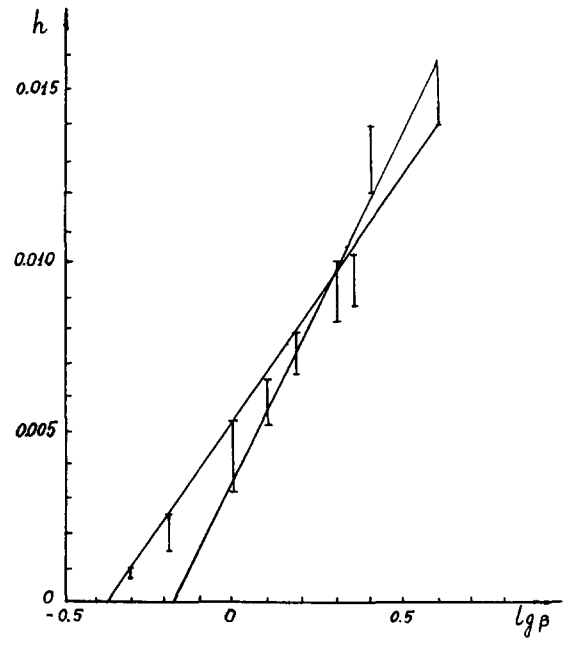

Fig. 2. Experimental dependence of KS entropy h (in $\sec^{-1}$) on β for the data of fig. 1.

Table 1

	N	K_0	E_0	ϵ_s		Ω/π	
				exp.	theor.	exp.	theor.
1	32	1, 3, 5	0.95	0.16	0.26	2.9×10^{-2}	3.1×10^{-2}
2 *	32	15, 17, 19	17	0.025	0.18	2.2×10^{-2}	3.1×10^{-2}
3 *	32	20	39	0.012	0.10	5×10^{-3}	3.1×10^{-2}
4	200	2	0.5	0.09	0.21	5×10^{-3}	5×10^{-3}
5	200	5	3	0.06	0.12	4×10^{-3}	5×10^{-3}
6	200	10	12	0.09	0.07	7×10^{-3}	5×10^{-3}
7	300	1	0.18	0.22	0.20	6×10^{-3}	3.3×10^{-3}
8	500	10	1.9	0.14	0.06	6×10^{-3}	2×10^{-3}
9 *	500	202	700	0.13	0.01	10^{-2}	2×10^{-3}

this region is found, after the energy equipartition, at about the border of stochasticity (3.1) whereas the value $\epsilon/\epsilon_s = 30$ in fig. 3 corresponds to the initial spectrum ($t = 0$, curve 1). The decline disappears by increasing ϵ.

(ii) The dying out of the autocorrelations (fig. 4) which is a direct indication of statistical relaxation.

(iii) The velocity distribution for chain particles (fig. 5) fits with good accuracy the one-dimensional maxwellian distribution: $dN/dv \propto \exp(-v^2/2T)$, where T is a "temperature" of the chain. This correspondence can be traced till the kinetic energy of the particle is almost five times the temperature. The "heat capacity" of the chain turns out to be (per degree of freedom): $G_1 = E_0/(N-1)T = 0.96$. The energy distribution for the oscillation modes obeys similarly the Gibbs law: $dN/dE_k \propto \exp(-E_k/T)$.

4. Stochasticity and solitons

Performed experiments would seem to resolve the FPU problem. The existence of the stochasticity border for a nonlinear chain as well as the statistical properties of the latter have also been confirmed independently by the numerical experiments of Japanese scientists [22]. Yet more careful analysis shows that we are still far from understanding the problem. One could even say that a new problem arises.

Indeed, as early as 1965 Kruskal and Zabusky ex-

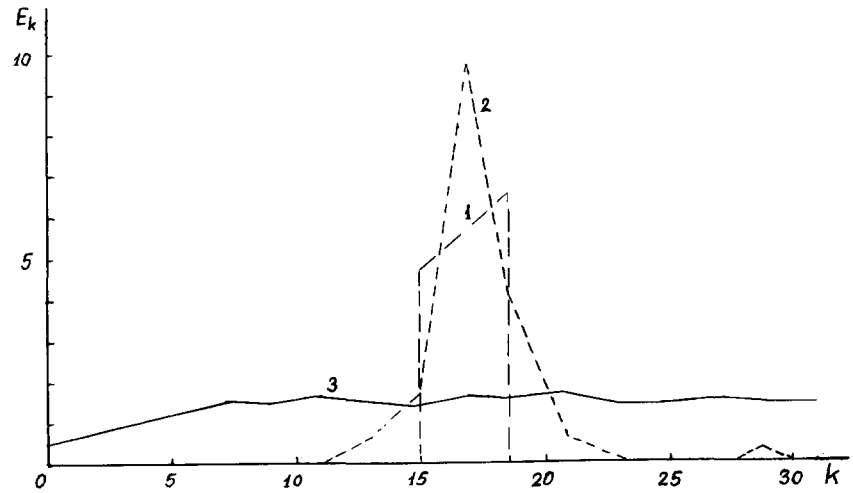

Fig. 3. Averaged spectrum of the energy of the mode for case 2 (see table 1): 1, initial excitation, $t = 0$; 2, $\epsilon/\epsilon_s \approx 2$ (initially), $t = 18\,300$; 3 – $\epsilon/\epsilon_s \approx 30$, $t = 16\,050$.

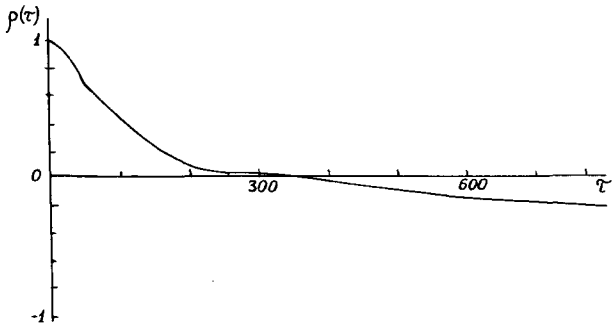

Fig. 4. Dying out of the autocorrelations of the 10th mode for case 6 (see table 1): $\epsilon/\epsilon_s \approx 12$.

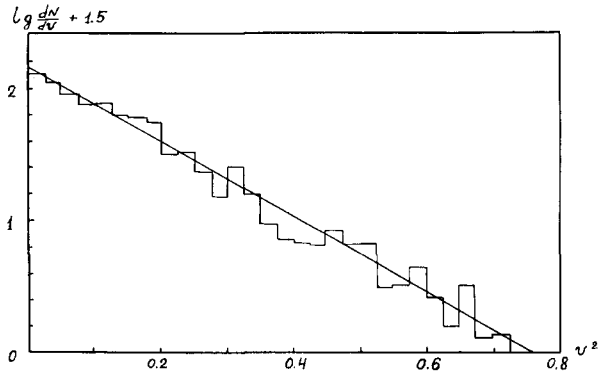

Fig. 5. Velocity distribution for particles of a nonlinear chain for case 6 (see table 1): $\epsilon/\epsilon_s \approx 8$; $E_0 = 14.76$; $E_{kin}/E_0 \approx 0.52$; $t = 3000$; the straight line is a maxwellian distribution with the "temperature" $T \approx 0.077$.

plained [15] the FPU result with the help of the remarkable stability, which they discovered, of the KdV equation. They showed by numerical experiments that the initial excitation decays into peculiar entities: solitons which reveal no interaction in spite of nonlinearity. So the problem arises concerning the correspondence of the KdV equation to the properties of a nonlinear chain which is alledgedly simulated by the former.

The main peculiarity of the KdV equation is that it describes the progressive wave only. Meanwhile all experiments with a nonlinear chain have dealt only with standing waves (ZBC). Therefore we have undertaken a number of experiments with periodic boudary conditions (PBC). It is true that we have failed to construct the initial excitation as a purely progressive wave, yet we managed to lower the share of the reverse wave down to a few per cent. In the latter case one could expect some increase in ϵ_s. But in reality ϵ_s even decreases a bit for PBC as compared with ZBC.

A typical picture of the motion in the stochastic region for PBC is given in fig. 6. A distinctive feature of the stochasticity development in this case is an abrupt rising of the reverse wave. Hence, the motion of the the nonlinear chain differs, in the end, qualitatively from that of KdV where the reverse wave is entirely impossible.

The question arises whether the reverse wave is the cause of stochasticity or its consequence. We think that the ultimate cause of stochasticity is related to the local instability which apparently gives rise to the reverse wave.

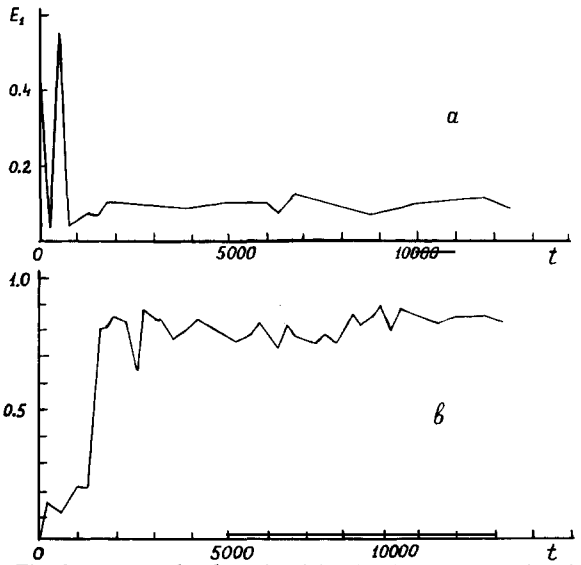

Fig. 6. An example of stochasticity development in a closed chain (PBC) for the initial excitation of the type of an almost progressive wave: (a) variation of the energy of the existed mode; (b) time dependence of the standing wave share; $N = 32$; $\epsilon/\epsilon_s \approx 1$.

For further investigation on this problem Toda's nonlinear chain with special interaction of neighbour particles is particularly suitable since the analytic expression for the purely progressive wave is known for this case [23].

5. Concluding remarks

As we have seen above, numerical experiments with the FPU model allow the study of a wide range of interesting mechanical problems. The possibility to trace the transition from discrete dynamical systems to continuous wave processes seems to us especially important. In particular, one can guess that the discovered statistical properties of the nonlinear chain take place, under certain conditions, for nonlinear waves as well. On the other hand, there are examples of integrable nonlinear wave equations (KdV and others, see for instance ref. [24]) for which the stochasticity is not possible. Exceptional as such cases apparently are, it would be natural to use them as the starting approximation for studying real wave processes. But the results of numerical experiments give no indication of any suppression of stochasticity by approaching such exceptional systems. For example, one would think that the properties of the chain should approach those of KdV, at least for progressive waves. Yet, this has not been observed in our numerical experiments. One could guess that case 9 in table 1 just shows such an anomaly (ϵ_s increases), but there are examples with a still smaller ϵ indicating no anomalies (for instance, cases 5 and 6; not to mention the cases 2 and 3). We think that clarifying this question is one of interesting lines of investigation in the field.

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