On stochastization of one-dimensional chains of nonlinear oscillators

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It is demonstrated that the inverse problem technique may be applied to the nonlinear string equation (2) and that the equation has an infinite set of commuting integrals of motion. The result is used to interpret the numerical experiments of Fermi, Pasta, and Ulam, who observed an anomalously slow stochastization of one-dimensional chains of nonlinear oscillators.

1. Fermi, Pasta, and Ulam performed in 1954 a series of numerical experiments aimed at ascertaining how randomization and the transition to a uniform energy distribution take place in dynamic systems with a large number of degrees of freedom[1,2]. The experiment were performed on one-dimensional chains of nonlinear oscillators representing discrete models of a nonlinear string. The nonlinearity level and the number of oscillators were large enough (the chain consisted of 64 oscillators in some experiments) for the experimenters to hope to discern rapid randomization of the chains and a transition to a uniform distribution of the energy over the degrees of freedom. They observed instead a quasiperiodic energy exchange between several initially excited modes and were unable to observe a tendency to a stochastic transition of the energy to higher modes over a sufficiently large time (up to several hundred oscillation periods).

The problem of anomalously slow randomization of one-dimensional chains of nonlinear oscillators is known as the "Fermi-Pasta-Ulam problem," and has recently been the subject of a number of studies, both analytic and based on results of numerical experiments (see the bibliography in the review[4]).

The most clearly pronounced "anomalous" behavior was demonstrated in the Fermi-Pasta-Ulam problem by a chain with a quadratic nonlinearity, the motion of which is described by the equations

$$\ddot{\xi}_i = \xi_{i+1} - 2\xi_i + \xi_{i-1} + (\xi_{i+1} - \xi_i)^2 - (\xi_i - \xi_{i-1})^2. \quad (1)$$

A regular quasiperiodic behavior of this chain was also observed later in detailed experiments by Deem and Zabusky[5].

The continual analog of chain (1) is a nonlinear string, the equation of which is conveniently written in the form

$$u_{tt} = u_{xx} + (u^2)_{xx} + {}^1/_4 u_{xxxx}. \quad (2)$$

We shall show in this paper that Eq. (2) has unique properties that can be used to explain the Fermi-Pasta-Ulam experiments. It must be emphasized from the very outset, however, that this explanation can be only qualitative, since we consider Eq. (2) with periodic boundary conditions, whereas in the numerical experiments the ends of the chains were regarded as fixed.

We shall show that Eq. (2) has an infinite set of integrals of motion that commute with one another. To this end, we rewrite Eq. (2) in the form of a system

$$u_t = \Phi_{xx}, \quad \Phi_t = u + u^2 + {}^1/_4 u_{xx} \quad (3)$$

and introduce two linear differential operators

$$\hat{L} = i\frac{d^3}{dx^3} + i\left(u\frac{d}{dx} + \frac{d}{dx}u\right) + i\frac{d}{dx} - \left(\frac{4}{3}\right)^{1/2}\Phi_x, \quad (4)$$

$$\hat{A} = \left(\frac{3}{4}\right)^{1/2}\frac{d^2}{dx^2} + \left(\frac{4}{3}\right)^{1/2}u. \quad (5)$$

It can be verified by direct substitution that the operator relation

$$\partial\hat{L}/\partial t = i(\hat{L}\hat{A} - \hat{A}\hat{L}) \quad (6)$$

is identical with the system (3).

We assume that Eq. (2) is specified on the interval $[0, l]$ with periodic boundary conditions at the ends of the interval, and consider the eigenvalue problem for the operator $\hat{L}$ on this interval:

$$\hat{L}\psi = \lambda\psi, \quad (7)$$

assuming likewise periodic boundary conditions for the function ψ. Differentiating (7) with respect to time and using (6), we obtain

$$(\hat{L} - \lambda)(\psi_t + i\hat{A}\psi) = \lambda_t\psi. \quad (8)$$

Taking the scalar product of (8) and ψ, and bearing (7) in mind, we obtain $\lambda_t = 0$. In other words, all the eigenvalues λ_i of the operator L are integrals of motion of Eq. (2). From (8) with $\lambda_t = 0$ it follows also that

$$\psi_t + i\hat{A}\psi = g(t)\psi. \quad (9)$$

Here g(t) is an arbitrary function of t and takes into account the fact that the normalization of the eigenfunction ψ can be varied arbitrarily with time.

2. We note that the system (3) can be expressed in Hamiltonian form:

$$u_t = -\frac{\delta H}{\delta \Phi}, \quad \Phi_t = \frac{\delta H}{\delta u}, \quad (10)$$

where

$$H = \int_0^l ({}^1/_2 u^2 + {}^1/_2 \Phi_x^2 + {}^1/_3 u^3 - {}^1/_8 u_x^2)\,dx$$

is the Hamiltonian of the system. This enables us to define for the functionals α and β of u and Φ the following Poisson brackets:

$$\{\alpha, \beta\} = \int_0^l \left(\frac{\delta\alpha}{\delta u}\frac{\delta\beta}{\delta\Phi} - \frac{\delta\alpha}{\delta\Phi}\frac{\delta\beta}{\delta u}\right)dx. \quad (11)$$

We shall show that the Poisson brackets between the eigenvalues λ_i of the operator $\hat{L}$ are equal to zero, and in this sense the λ_i are commuting integrals of motion of the system (3). The variation $\delta\lambda$ of the eigenvalue λ following an infinitesimally small perturbation $\delta\hat{L}$ of the operator $\hat{L}$ is given by

$$\delta\lambda = \langle\psi|\delta\hat{L}|\psi\rangle. \quad (12)$$

Here ψ is an eigenfunction of the operator $\hat{L}$ and satisfies the equation

$$i\psi_{xxx}+i(2u+1)\psi_x+iu_x\psi-(4/3)^{1/2}\Phi_x\psi=\lambda\psi. \qquad (13)$$

From (4) we have

$$\delta\hat{L}=i\left(\delta u\frac{d}{dx}+\frac{d}{dx}\delta u\right)-\left(\frac{4}{3}\right)^{1/2}(\delta\Phi)_x. \qquad (14)$$

Substituting (14) in (12) we find

$$\frac{\delta\lambda}{\delta u}=i(\psi^*\psi_x-\psi\psi_x^*),\quad \frac{\delta\lambda}{\delta\Phi}=\left(\frac{4}{3}\right)^{1/2}\frac{d}{dx}|\psi|^2. \qquad (15)$$

We introduce a symbol for the arbitrary functions χ_1 and χ_2:

$$[\chi_1,\chi_2]=\chi_1\chi_{2x}-\chi_2\chi_{1x}.$$

From (11) and (15) we obtain for the two eigenvalues λ_1 and λ_2:

$$\{\lambda_1,\lambda_2\}=\left(\frac{4}{3}\right)^{1/2}i\int_0^l\left([\psi_1^*,\psi_1]\frac{d}{dx}|\psi_2|^2-[\psi_2^*,\psi_2]\frac{d}{dx}|\psi_1|^2\right)dx$$

$$=\left(\frac{4}{3}\right)^{1/2}i\int_0^l\left(\psi_1\psi_2\frac{d}{dx}[\psi_2^*\psi_1^*]-\psi_1^*\psi_2^*\frac{d}{dx}[\psi_2,\psi_1]\right)dx. \qquad (16)$$

Here ψ_1 and ψ_2 are the corresponding eigenfunctions. It is easy to obtain from (13) the relations

$$\psi_1\psi_2=\frac{i}{\lambda_1-\lambda_2}\left\{\frac{d^2}{dx^2}[\psi_2,\psi_1]-[\psi_{2x},\psi_{1x}]+(2u+1)[\psi_2,\psi_1]\right\}, \qquad (17)$$

$$\frac{d}{dx}[\psi_{2x},\psi_{1x}]=u_x[\psi_2,\psi_1]+i\left(\frac{4}{3}\right)^{1/2}\Phi_x[\psi_2,\psi_1]+i(\lambda_2\psi_2\psi_{1x}-\lambda_1\psi_1\psi_{2x}). \qquad (18)$$

Substituting (17) in (16) and using (18), we obtain after simple transformations

$$\{\lambda_1,\lambda_2\}=-\left(\frac{4}{3}\right)^{1/2}\frac{i}{\lambda_1-\lambda_2}\int_0^l\{[\psi_2^*,\psi_1^*](\lambda_2\psi_2\psi_{1x}-\lambda_1\psi_1\psi_{2x})$$
$$-[\psi_2,\psi_1](\lambda_2\psi_2^*\psi_{1x}^*-\lambda_1\psi_1^*\psi_{2x}^*)\}dx.$$

Putting $\lambda_1 = a + b$ and $\lambda_2 = a - b$, we get

$$\{\lambda_1,\lambda_2\}=\left(\frac{4}{3}\right)^{1/2}\frac{b}{\lambda_1-\lambda_2}\int_0^l\left\{[\psi_2^*,\psi_1^*]\frac{d}{dx}\psi_2\psi_1\right.$$
$$\left.-[\psi_2,\psi_1]\frac{d}{dx}\psi_2^*\psi_1^*\right\}dx=-\frac{1}{2}\{\lambda_1,\lambda_2\},$$

from which it follows that $\{\lambda_1, \lambda_2\} = 0$.

3. In addition to the integrals λ_i we can obtain an infinite set of "polynomial" integrals of the motion, which are expressed explicitly in terms of the "field" variables u and Φ. To this end we assume that a certain solution ψ of Eq. (13) satisfies the condition $\psi(l) = e^{ikl}$ and consequently admits of a representation in the form

$$\psi=\exp\left\{ikx+i\int_x^l\chi(x,k)dx\right\}, \qquad (19)$$

where k is a real root of the equation $k^3 - k = \lambda$. Substituting (19) in (9) and (13) we obtain

$$\frac{d\chi}{\partial t}=-\frac{\partial}{\partial x}\left\{\left(\frac{3}{4}\right)^{1/2}(i\chi_x+\chi^2-2k\chi)-\left(\frac{4}{3}\right)^{1/2}u\right\}, \qquad (20)$$

$$\chi=\frac{1}{k}\left(\chi^2+i\chi_x-\frac{2}{3}u\right)+$$
$$+\frac{1}{3k^2}\left(\chi_{xx}-3i\chi\chi_x-\chi^3+(2u+1)\chi+iu_x-\left(\frac{4}{3}\right)^{1/2}v\right). \qquad (21)$$

Here $v = \Phi_x$. It follows directly from (20) that the quantity

$$\chi(k)=\int_0^l\chi(x,k)dx$$

is conserved in time.

We consider the asymptotic form of $\chi(x, k)$ at large values of k:

$$\chi(x,k)\approx\sum_{n=1}^{\infty}\frac{\chi_n(x)}{k^n}. \qquad (22)$$

Accordingly

$$\chi(k)\approx\sum_{n=1}^{\infty}\frac{I_n}{k^n},\quad I_n=\int_0^l\chi_n(x)dx. \qquad (23)$$

All the I_n are integrals of motion of the system (3). Substituting (22) in (21) and (20) we obtain the recurrence formulas

$$\chi_{n+1}=i\chi_{nx}+\sum_{k=1}^{n}\chi_k\chi_{n-k}+{}^1/_3(\chi_{n-1})_{xx}-\sum_{k=1}^{n-2}\chi_k(\chi_{n-k-1})_x$$
$$-{}^1/_3\sum_{i+j+l=n-1}\chi_i\chi_j\chi_l+{}^1/_3(2u+1)\chi_{n-1}\qquad(n>2), \qquad (24)$$
$$\chi_1=-{}^2/_3u,\quad \chi_2=-{}^1/_3(iu_x+({}^4/_3)^{1/2}v).$$

Here

$$\partial\chi_n/\partial t=\partial\eta_n/\partial x,\quad \eta_n=({}^3/_4)^{1/2}\left(i\chi_{nx}+\sum_{k=1}^{n-1}\chi_k\chi_{n-k}-2\chi_{n+1}\right),$$
$$\eta_1=({}^3/_4)^{1/2}(i\chi_{1x}-2\chi_2-{}^3/_4u). \qquad (25)$$

Formulas (23)–(25) enable us to find all the I_n. We present the first seven:

$$I_1=-{}^2/_3\int_0^l u\,dx,\quad I_2=-{}^1/_3({}^4/_3)^{1/2}\int_0^l v\,dx,$$

$$I_3={}^1/_3I_1,\quad I_4={}^2/_9({}^4/_3)^{1/2}\int_0^l uv\,dx+{}^1/_3I_2,$$

$$I_5={}^8/_{27}\int_0^l({}^1/_2u^2+{}^1/_2v^2+{}^1/_3u^3-{}^1/_8u_x^2)dx+{}^1/_9I_1, \qquad (26)$$

$$I_6={}^4/_3I_4-{}^1/_3I_2,$$

$$I_7=-{}^1/_{81}\int_0^l(u_{xx}^2-4v_x^2+16uv^2-12u_x^2u+{}^{16}/_3u^4-2u_x^2-8u_x^2-8v^2)dx.$$

It follows from (26) that not all the I_n are independent; thus, I_3 and I_6 are expressed in terms of the lower integrals. The first three independent integrals I_1, I_2, and I_4 follow directly from the system (3), and the integral I_5 is expressed in terms of the Hamiltonian:

$$I_5={}^8/_{27}H+{}^1/_9I_1.$$

The first nontrivial integral is I_7.

4. For a Hamiltonian system with a finite number N, of degrees of freedom, the existence of N commuting integrals of motion means, by virtue of the Liouville theorem (see, e.g.,[6]), that the system is fully integrable, i.e., that it is possible to separate the variables and to introduce action and angle variables. The integrable systems are not completely randomized, since there is no exchange of energy between the degrees of freedom.

For a Hamiltonian system with a denumerable number of degrees of freedom, such as Eq. (2) with periodic boundary conditions, the existence of a denumerable set of commuting integrals is only the necessary condition of integrability, and it is still necessary to prove the "completeness" of this set. If, however, we take the position that Eq. (2) is a fully integrable system, then the results of the Fermi-Pasta-Ulam experiments become naturally explicable.

The possible cause of randomization of the chain (1) in this case is not the level of its nonlinearity, but the degree of its deviation from a fully integrable continual limit.

For the smooth initial conditions considered in the Fermi-Pasta-Ulam experiments, this deviation is of the order of $\xi''/\xi \sim 1/N^2$, where N is the number of oscillators in the chain. At N = 64 this leads to a decrease of the "effective nonlinearity" by a factor 10^3–10^4 and to a corresponding increase of the randomization time to values by far not attained in the numerical experiments. When the number of oscillators in the chain is increased, the randomization time becomes correspondingly more remote.

5. The fact that the system (3) is identical with the operator relation (6) means that the method of the inverse problem can be applied to the system (3)[7-10]. This method was applied earlier to the Korteveg-deVries equation[7,8]

$$u_t + uu_x + u_{xxx} = 0 \qquad (27)$$

and to the nonlinear "parabolic" equation[9,10]

$$i\psi_t + \psi_{xx} \pm |\psi|^2 = 0. \qquad (28)$$

The role of the operator L is assumed in these equations by the one-dimensional Schrodinger operator and the one-dimensional Dirac operator, respectively. It is of interest to compare the results obtained for Eqs. (27) and (28) with our present results.

In the case of periodic boundary conditions, there is a complete analogy between the results. For Eqs. (27) and (28) it is possible to establish the existence of sets of commuting integrals of the eigenvalues of the corresponding operators and to calculate the polynomial conservation laws. No proof of the existence of these sets for Eqs. (27) and (28) has been obtained as yet.

In the case of these equations, however, it is possible to make considerable progress by assuming zero conditions as $|x| \to \infty$. In this case, complete integrability was proved in[11], and the interaction of particular solutions of the equations, corresponding to discrete levels of the spectra (solitons) was investigated[8-10,12]. These results are based on the formalism of the inverse scattering problem for the corresponding operators $\hat{L}$. They can probably be extended also to include Eq. (2), although the construction of the theory of the inverse scattering problem for the third-order operator (4) is a difficult and as yet unsolved mathematical problem.

In conclusion, we make one more remark with respect to randomization of the one-dimensional Hamiltonian systems of general type. Among the one-dimensional Hamiltonian systems there exist apparently many fully-integrable ones, many of which remain unclassified and unlisted to this day. When a given Hamiltonian system is studied, it must be borne in mind that the rate of its randomization is determined by the degree to which the system is close to the nearest fully integrable system. Accidental causes can make this "distance" small (as was apparently the case with chain (1)), and this increases the randomization time.

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