PHYSICAL REVIEW LETTERS

VOLUME 37 12 JULY 1976 NUMBER 2

Explanation of Instabilities Observed on a Fermi-Pasta-Ulam Lattice*

C. F. Driscoll and T. M. O'Neil
University of California at San Diego, La Jolla, California 92037
(Received 29 April 1976)

Exponential instability of waves on the cubically nonlinear, one-dimensional lattice is considered. The lattice has been modeled by the modified Korteweg–de Vries (mKdV) equation. It is shown that some solutions of the mKdV equation are unstable, and that these mKdV instabilities correspond to the instabilities observed on the lattice. Such instabilities may be important in determining whether or not a system behaves stochastically.

Fermi, Pasta, and Ulam (FPU) attempted to relate nonlinear dynamics to the ergodic hypothesis by numerical simulation of one-dimensional lattices with nonlinear restoring forces.[1] They expected randomization and equipartition of energy among Fourier modes, but instead found periodic recurrences of modal energies.

Zabusky and Kruskal[2] explained these recurrences as echos due to essentially free-streaming nonlinear pulses, or solitons. They approximated the discrete lattice system by the continuum Korteweg–de Vries (KdV) equation for quadratic nonlinearity, and by the modified Korteweg–de Vries (mKdV) equation for cubic nonlinearity. General initial conditions were observed to break up into solitons which maintained their individual identities even after nonlinear interaction. Two mathematical frameworks, the inverse-scattering method of Gardner *et al.*[3] and the Bäcklund transformation of Wahlquist and Estabrook,[4] have been developed to solve the KdV and mKdV equations analytically.

Since the work of FPU, the physical basis of ergodic theory has been developed considerably. Dynamical systems have been found which are ergodic and mixing, and Anosov and Sinai[5] have shown the essential feature of such systems to be local instability in phase space; that is, two arbitrarily close initial conditions separate exponentially with time. Ford[6] and co-workers have demonstrated that systems may be unstable in certain stochastic regions of phase space while not globally ergodic.

Several groups have attempted to understand the local instability properties of the cubically non-linear FPU lattice. Bivins *et al.*[7] related the lattice instability to that of a Mathiue equation for singular initial conditions. Izrailev and Chirikov[8] have attempted to establish a "stochastic limit" for the lattice, based on the concept of resonance overlap. Since solutions of the mKdV equation have been thought to be stable, the relevance of the mKdV equation to the lattice system has been questioned.[8]

In this Letter, we show that the mKdV equation correctly models the instabilities on the cubically nonlinear FPU lattice; the explanation is based on the recent theoretical observation[9] that certain solutions of the mKdV equation are unstable. Since general initial conditions form solitons, we start with a cnoidal wave train, i.e., the periodic generalization of solitons. The stability properties of mKdV cnoidal waves are determined by application of Whitham's modulational theory,[10] and by numerical solution of the linearized eigenvalue problem. We then excite these cnoidal waves on the FPU lattice, and numerically integrate the dynamics to determine the lattice stability. We find that the lattice and mKdV growth rates agree for large numbers of lattice masses; that is, the lattice instability is modeled by the mKdV equation.

The one-dimensional, cubically nonlinear lattice is governed by the dynamical equation

$$\partial^2 y_j/\partial t^2 = (y_{j+1} - y_j) - (y_j - y_{j-1}) \pm \tfrac{1}{3}[(y_{j+1} - y_j)^3 - (y_j - y_{j-1})^3]. \qquad (1)$$

Here, $y_j(t)$ is the displacement from equilibrium of the jth mass, $j = 1, 2, \ldots, N$, and periodic boundary conditions are specified by $y_0 = y_N$ and $y_{N+1} = y_1$. The nonlinear coefficient $\frac{1}{3}$ may be rescaled to any value, but the choice of sign represents two distinct dynamical possibilities which will be considered explicitly. Following Zabusky,[2] we consider the lattice displacement to be a continuous function $y(x,t)$, with $y(jh,t) = y_j(t)$, where $h \equiv L/N$, and L is the system length. Define the variable $u(x,t)$ representing waves traveling in the positive direction as

$$u \equiv -y_t/2h + \tfrac{1}{2}\int_0^{y_x} (1 \pm h^2\eta^2)^{1/2}\, d\eta, \qquad (2)$$

where the subscript x or t denotes partial differentiation. The discrete differences in Eq. (1) are expressed as Taylor expansions, and only lowest-order terms in dispersion and nonlinearity are kept. Then, ignoring coupling to waves traveling in the negative direction, one obtains the mKdV equation

$$u_\tau \pm 12u^2 u_\xi + u_{\xi\xi\xi} = 0, \qquad (3)$$

where $\xi \equiv x - ht$ and $\tau \equiv h^3 t/24$. The KdV equation, representing quadratically nonlinear systems, would have the nonlinear term uu_ξ instead of $u^2 u_\xi$.

The periodic solutions of Eq. (3) stationary in the frame $\xi - C\tau$ may be obtained by integrating Eq. (3) twice. This gives

$$\tfrac{1}{2}u_\xi^2 \pm u^4 - \tfrac{1}{2}Cu^2 + Bu + A \equiv \tfrac{1}{2}u_\xi^2 + \mathcal{P}(u) = 0, \qquad (4)$$

where A and B are constants of integration. Since the "oscillator" polynomial $\mathcal{P}(u)$ is fourth order, the solution of Eq. (4) may be expressed in terms of the Jacobian elliptic functions,[11] e.g., $\mathrm{cn}(\xi, q)$, and is called a cnoidal wave. The cnoidal wave is determined by the three parameters A, B, and C, or equivalently by the roots a, b, c, and d of $\mathcal{P}(u)$, with $a+b+c+d=0$ from Eq. (4).

Since $u \simeq y_x$ for small h, a periodic cnoidal wave u will give a periodic lattice displacement y only if the spatial mean of u is zero. For comparison with the lattice, we thus consider only those cnoidal waves with $B=0$, symmetric in positive and negative u, which consequently have zero mean. Furthermore, since the length L introduced in Eq. (2) is arbitrary, we need only consider cnoidal waves with wavelength $\lambda = 1$, i.e., wave number $k = 2\pi$. With these two restrictions, the cnoidal waves are described by a single parameter, which we choose to be the cnoidal modulus q, $0 \le q < 1$. For small q, the waves are small amplitude and almost sinusoidal; for q near 1, the waves are large-amplitude, well-separated solitons.

The stability of mKdV cnoidal waves with respect to long-wavelength perturbations may be obtained using Whitham's modulational theory.[10] The waves are found to be stable if all four roots of the associated polynomial $\mathcal{P}(u)$ are real, and unstable if two roots are real and two are complex.[9] For the mKdV equation (3) with *negative* sign choice, all cnoidal wave solutions are stable, since the polynomials $\mathcal{P}(u)$ associated with bounded solutions all have four real roots. For the mKdV equation (3) with *positive* sign choice, some cnoidal wave solutions are unstable, corresponding to polynomials $\mathcal{P}(u)$ with two real and two complex roots. The $B=0$, zero-mean cnoidal waves which we consider here are unstable for this sign choice. The exponential instability rate for these waves may be expressed as

$$\gamma = \frac{32q(1-q^2)^{1/2}K^3[q^2E + (1-q^2)(K-E)]}{q^2E^2 + (1-q^2)(K-E)^2}\,\kappa. \qquad (5)$$

Here, κ is the wave number of the perturbation, and $K(q)$ and $E(q)$ are the complete elliptic integrals of the first and second kinds.[11]

The growth rate of Eq. (5) is valid only for long-wavelength perturbations, i.e. $\kappa/k \ll 1$. To obtain stability predictions for shorter-wavelength perturbations, we have employed two further methods. First, for small-amplitude cnoidal waves, mode-coupling theory[10] gives corrections of higher order in κ/k; these determine the maximum unstable perturbation wave number to be $\kappa/k \simeq q$, for small q. Second, we determine the unstable modes of any given cnoidal wave u_0 by numerically solving the linearized eigenvalue problem

$$i\nu v - Cv_\xi \pm 12(u_0^2 v)_\xi + v_{\xi\xi\xi} = 0, \qquad (6)$$

where $u(\xi,\tau) = u_0(\xi) + v(\xi)\exp(i\nu\tau)$. We solve Eq. (6) in Fourier space, keeping only a finite number of modes. The linear transformation on v is then represented by a matrix determined by C and the Fourier modes of u_0. We find the eigenvalues ν and eigenvectors v of this matrix using the numerical routines of EISPACK.[12] The numerical eigenvalue results agree with the analytic results and can be extended to large κ/k and q. The instability results for the positive sign choice in Eq. (3) are summarized in Fig. 1; here, we display the growth rate $\gamma = \text{Im}(\nu)$ vs κ/k and q^2, with two cross sections at $\kappa/k = \frac{1}{2}$ and 1.

We now relate these instability results to the discrete lattice. A given cnoidal wave $u(\xi)$ can be excited on the lattice by constructing displacement and velocity functions $y(x, 0)$ and $y_t(x, 0)$ that correspond to $u(\xi)$ through Eq. (2). The functions y and y_t are constructed from positively traveling Fourier modes of the lattice by an iterative convergent procedure. For large N, the mass displacements and velocities y_j and y_{jt} will accurately represent the cnoidal wave; for small N, the representation will be more approximate.

Starting from the cnoidal-wave initial conditions, we numerically integrate the lattice dynamical equation (1) forward in time, using Scranton's algorithm.[13] The cnoidal wave is observed to move with constant form and velocity, and its modal energies remain constant. Those modes not present in the cnoidal wave have only noise initially present; but for unstable waves, these modes grow exponentially. We characterize the growth by its exponentiation time t_e. If these modes initially had precisely zero amplitude, the dynamical symmetry would require that they always have zero amplitude; their growth represents two initially close phase-space points separating exponentially. The correspondence with the mKdV equation is made by calculating the scaled exponentiation time $\tau_e \equiv t_e h^3/24$, or equivalently the scaled growth rate $\gamma \equiv 1/\tau_e$.

Lattice-instability results for the positive sign in Eq. (1) are shown in Fig. 2. In Fig. 2(a) we excite cnoidal waves with wavelength $\lambda = 1$ (parametrized by q) on the lattice with periodicity length $L = 2$; that is, there are two complete cnoidal waves on the lattice of N masses. We observe the exponential growth from noise of the lattice mode with length 2. This corresponds to the mKdV modulational instability with $\kappa/k = \frac{1}{2}$, shown as a cross section in Fig. 1 and as the solid curve in Fig. 2(a). The data points of Fig. 2(a) are the scaled lattice instability rates γ for various N. The uncertainty in the determination of γ is approximately ± 5%. The lattice growth

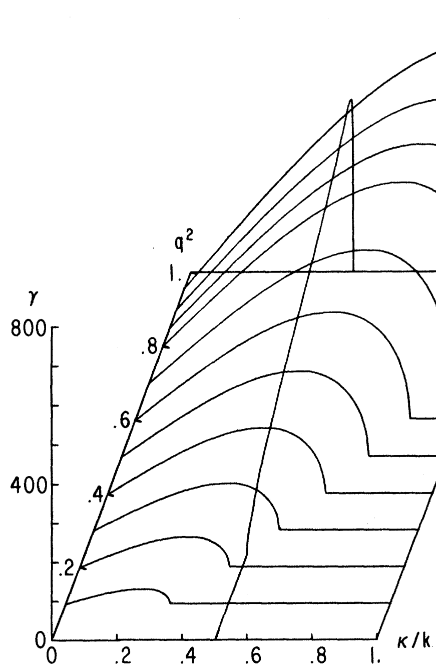

FIG. 1. mKdV cnoidal-wave instability rate γ versus scaled perturbation wave number κ/k and wave modulus q^2.

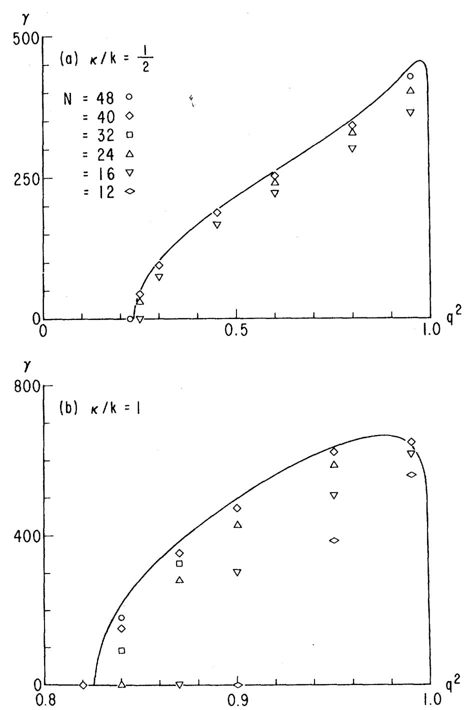

FIG. 2. Scaled lattice instability rate γ (data points) and mKdV prediction (solid curve) for cnoidal waves with modulus q^2. (a) Growth of longer-wavelength mode. (b) Growth of forbidden modes.

rates are seen to asymptotically approach the mKdV prediction, as N becomes large.

In Fig. 2(b) we excite cnoidal waves with $\lambda = 1$ on the lattice with periodicity length $L = 1$; that is, there is one complete wave on the lattice of N masses. Growth of longer-wavelength modes is prevented by the periodic boundary conditions. The "forbidden modes" $2k$, $4k$, etc., are not present in the cnoidal wave, since the cubic nonlinearity couples mode k only to its odd harmonics. These forbidden modes are, however, observed to grow exponentially from noise. This corresponds to the mKdV instability with $\kappa/k = 1$. We measure the exponential growth of mode $2k$, and plot the scaled growth rate γ. Again, we observe that the lattice instability for large N agrees with the mKdV prediction.

The $\kappa/k = 1$ instability is seen to be quenched for $q^2 < 0.826$, as is the $\kappa/k = \frac{1}{2}$ instability for $q^2 < 0.235$. Thus the "instability limit" for cnoidal waves depends on the boundary conditions imposed. Any given cnoidal wave (modulus q, $\lambda = 1$) will become unstable as the periodic system is made "longer," i.e., as longer-wavelength perturbations are allowed. We also observe an instability limit as N is decreased; this limit is not, of course, contained in the mKdV equation.

For the lattice with negative nonlinear term in Eq. (1), we observe no exponential instability; this corresponds to the stability of cnoidal-wave solutions of the mKdV equation with negative nonlinear term. This lattice is, however, subject to explosive dissociation, since for large displacements the potential energy may become infinitely negative.

When general (e.g., sinusoidal) initial conditions are imposed on the lattice, solitons are observed to form and stream through one another. Fourier modes which initially have almost zero amplitude are observed to grow in an irregular, but basically exponential, manner. Since the "zeroth-order" configuration is changing with time as the solitons stream through one another, a "first-order" stability analysis would be difficult. We find, however, that the scaled lattice growth rate $\gamma(N)$ approaches a constant for large N, and this rate is consistent with the instability of cnoidal waves of appropriate amplitude and wave number.[14] Thus we see that the lattice instability from sinusoidal initial conditions is also modeled by the mKdV equation and is similar to the instability observed for cnoidal waves. These instability results do not agree with the predictions of the resonance-overlap model,[8] differing in the dependence on N and on the initial excitation amplitude.

The lattice instabilities have been interpreted as signaling the onset of stochastic behavior[8]; yet the instabilities are modeled by the mKdV equation which is known to have an infinite number of integral invariants.[15] Further analytic study of the mKdV equation may clarify the nature of these instabilities and provide a link between the work on stochastic systems with few degrees of freedom[6] and similar nonlinear systems with many degrees of freedom.

*Work supported by National Science Foundation Grant No. PHY-73-05125-A02 and Alfred P. Sloan Grant No. BR-1323.

[1] E. Fermi *et al.*, Los Alamos Scientific Laboratory Report No. LA-1940, 1955 (unpublished).

[2] N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. 15, 240 (1965); N. J. Zabusky, in *Nonlinear Partial Differential Equations*, edited by W. F. Ames (Academic, New York, 1967), p. 223.

[3] C. S. Gardner *et al.*, Phys. Rev. Lett. 19, 1095 (1967).

[4] H. D. Wahlquist and F. B. Estabrook, Phys. Rev. Lett. 31, 1386 (1973).

[5] D. V. Anosov and Ya. G. Sinai, Russ. Math. Surveys 22, No. 5, 103 (1967).

[6] J. Ford, Adv. Chem. Phys. 24, 155 (1973).

[7] R. L. Bivins *et al.*, J. Comput. Phys. 12, 65 (1973).

[8] F. M. Izrailev and B. V. Chirikov, Dokl. Akad. Nauk 166, 57 (1966) [Sov. Phys. Dokl. 11, 30 (1966)]; B. V. Chirikov *et al.*, Comput. Phys. Commun. 5, 11 (1973).

[9] C. F. Driscoll and T. M. O'Neil, to be published.

[10] G. B. Whitham, *Linear and Nonlinear Waves* (Wiley, New York, 1974), Sects. 16.14 and 15.6.

[11] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965), Sects. 8.1 and 3.147.

[12] B. T. Smith *et al.*, *Matrix Eigensystem Routines—EISPACK Guide* (Springer, Heidelberg, 1976).

[13] R. E. Scranton, Comput. J. 6, 386 (1964).

[14] C. F. Driscoll and T. M. O'Neil, to be published.

[15] R. M. Miura *et al.*, J. Math Phys. (N.Y.) 9, 1204 (1968).