Modulational instability of travelling waves in Fermi–Pasta–Ulam lattices

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The modulational instability of traveling waves in monatomic lattices with quartic anharmonicity is studied analytically and numerically. It is shown that the waves of the middle of the Brillouin zone are very unstable and that additional regions corresponding to waves propagating in the opposite direction appear for them in the space of perturbative wave vectors along with the usual modulational-instability region. A strong dependence of the recurrence phenomenon on the wave vectors of the dominant wave and the perturbative wave is discovered.

1. INTRODUCTION

The investigation of the stability of wave processes in nonlinear systems has been the subject of an extensive list of publications owing to the major role which stable and decaying nonlinear excitations play in various areas of physics. One special case of the instability of a wave process is the modulational instability.[1–3] Its essential feature is that the amplitude of a wave in a nonlinear medium is unstable with respect to spatial and/or temporal modulation. Spatiotemporal Fourier analysis of a process with evolving modulational instability reveals not only the dominant harmonic, but also additional equally spaced satellite components, whose amplitudes increase exponentially in the initial stage of evolution. On long time scales a process controlled by modulational instability is periodic, i.e., the conversion of the energy of the dominant wave into the energy of satellites is followed by its return to the dominant wave. The intermediate stage is associated with a spatial distribution of the energy that is characteristic of a train of solitons. It has been suggested that this property of the modulational instability of plane waves can serve as a mechanism for generating ultrashort light pulses in nonlinear fibers.[4]

The modulational instability of waves is organically related to the possibility of the existence of soliton-like excitations and has been investigated in great detail in reference to continuum nonlinear systems. At the same time, recent investigations of discrete systems, in which modulational instability has been studied to a small extent, have revealed the existence of strongly localized modes, which are specific to discrete structures.[5–8] For example, the modulational instability observed in a one-dimensional lattice containing only a narrow optical branch of excitations (a Klein–Gordon lattice) was analyzed in Ref. 9, where it was shown that its characteristic feature is a dependence of the instability region on the wave vector of the carrier wave.

To ascertain the influence of the modulational instability on processes occurring in real physical systems, departure from the approximation associated with consideration of a narrow optical branch of excitations is clearly necessary. In this sense monatomic lattices with a potential due to the interaction of neighboring particles containing third- and fourth-order anharmonic terms are good model systems. Such lattices are often used to study the modal and transport properties of real crystals. Using such lattices, in the mid-fifties Fermi, Pasta, and Ulam discovered the phenomenon of a periodic time dependence of the distribution function of the energy among spatial modes, which is presently known as Fermi–Pasta–Ulam (FPU) recurrence.[10] Since that time the problem of FPU recurrence and the study of the dynamic properties of these lattices, which are often called Fermi–Pasta–Ulam lattices, have been the subject of numerous publications (see, for example, Refs. 11–13 and the literature cited therein). In particular, in contrast to Ref. 10, the temporal evolution of the higher (short-wavelength) modes of a lattice was studied in Refs. 11 and 12, and the instability of these modes, as well as a recurrence phenomenon similar to FPU recurrence for the lower (long-wavelength) modes, were discovered. We note that standing waves were investigated in lattices with fixed end particles in Refs. 10–13. At the same time, traveling waves are of very great interest from the point of view of studying the transport properties of ultrashort pulses and processes which generate them.

The present work is devoted to an analysis of the modulational instability of traveling waves in FPU lattices with quartic anharmonicity (the influence of the cubic anharmonicity on modulational instability can be taken into account by renormalizing the quartic anharmonicity constant). We shall demonstrate analytically and confirm in a numerical experiment that, in contrast to the modulational instability in the known continuum and discrete models, two additional regions of modulational instability, which exist for any sign of the quartic nonlinearity and correspond to the generation of perturbative waves that propagate mainly toward the carrier wave, appear in FPU lattices. It follows from our analysis that excitations of the middle of the Brillouin zone are the most unstable (in the sense of global instability).

2. THEORY

The equations of motion of particles in a monatomic lattice with quartic anharmonicity have the form

$$\ddot{U}_n+K_2(2U_n-U_{n-1}-U_{n+1})+K_4[(U_n-U_{n-1})^3+(U_n-U_{n+1})^3]=0, \tag{1}$$

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in which U_n denotes the displacement of the nth particle from the equilibrium position and K_2 and K_4 are the linear and nonlinear force constants.

In the long-wavelength limit this equation for waves moving in one direction reduces to a modified Korteweg–de Vries equation, which belongs to a class of fully integrable equations and has, in particular, soliton solutions. In the short-wavelength limit, where the wave vector of the carrier wave lies near the boundary of the Brillouin zone, the so-called semidiscrete approximation, which makes it possible to describe the amplitude of the envelope in the continuum approximation, is usually used.[14] We shall not employ passage to any continuum approximation, and we shall take into account the discrete nature of the lattice exactly in the context of Eq. (1).

In the single-particle (rotating-wave) Eq. (1) has a solution of the form

$$U_n(t)=\tfrac{1}{2}(V_0\exp[i(\omega t-kn)]+\text{c.c.}), \tag{2}$$

where

$$\omega^2=4K_2\sin^2\left(\frac{k}{2}\right)+12K_4|V_0|^2\cdot\sin^4\left(\frac{k}{2}\right), \tag{3}$$

and k is the wave vector in units of the reciprocal lattice constant. With no loss of generality we can henceforth assume that V_0 is a real quantity.

To analyze the stability of the solution (2), we substitute the perturbed value of the amplitude $V_0+\Psi_n(t)$, where $|\Psi_n|\ll V_0$, into (1). The linearized equation for $\Psi_n(t)$ has the form

$$\begin{aligned}\omega^2\Psi_n-\ddot{\Psi}_n-2i\omega\dot{\Psi}_n+\tilde{K}_2(\Psi_{n+1}e^{-ik}+\Psi_{n-1}e^{ik}\\ -2\Psi n)-2\tilde{K}_4(\Psi^*_{n+1}+\Psi^*_{n-1}\\ -2\Psi^*_n\cos k)=0,\end{aligned} \tag{4}$$

where $\tilde{K}_2=K_2+4\tilde{K}_4$ and $\tilde{K}_4=(3/2)K_4V_0^2\sin^2(k/2)$.

Then setting $\Psi_n=A\exp[i(Qn-\Omega t)]+B\exp[-i(Qn-\Omega t)]$ and following the standard procedure for the linear analysis of stability, we obtain the following equation, which specifies the function $\Omega(k,Q)$:

$$\begin{aligned}&\{(\omega+\Omega)^2-4\tilde{K}_2\sin^2[(k+Q)/2)]\}\\ &\times\{(\omega-\Omega)^2-4\tilde{K}_2\sin^2[(k-Q)/2]\}\\ &=[4\tilde{K}_4(\cos k-\cos Q)]^2.\end{aligned} \tag{5}$$

It follows from (5) that for a given k there are ranges of values of Q in which the roots of Eq. (5) become complex. This signifies modulation instability of the solution of Eq. (1) in the form of a traveling wave, which is manifested by the exponential growth of satellite components, i.e., waves with the wave vectors $k\pm Q$.

An analysis reveals that of the four roots of Eq. (5), Ω_3 and Ω_4 are always real and that $|\Omega_3|\approx|\Omega_4|\approx 2\omega$ for $k\pm Q\neq 2\pi n$. These two roots correspond to solutions in the region of the third harmonic, in which we are not interested, especially since a proper analysis of the solution in that frequency range requires departure from the single-particle approximation used. The other two roots, $|\Omega_1\approx|\Omega_2|<\omega$ can have either real or complex values. The condition $|\Omega_3|\approx|\Omega_4|\gg|\Omega_1|\approx|\Omega_2|$ allows us to write down an approximate formula for the roots of Eq. (5) of interest to us and consequently to derive an expression for the imaginary part of the frequency $\Omega=\Omega'+i\Omega''$:

$$\Omega''\cong\pm\frac{1}{2}\left[\frac{[16\tilde{K}_4(\cos k-\cos Q)]^2}{(2\omega+3\delta_- -\delta_+)(2\omega+3\delta_+ -\delta_-)}-(2\omega-\delta_+-\delta_-)^2\right]^{1/2}, \tag{6}$$

where

$$\delta_\pm=2\sqrt{\tilde{K}_2}\left|\sin\left(\frac{k\pm Q}{2}\right)\right|. \tag{7}$$

Modulation instability occurs for the values of the wave vectors k and Q, such that the radical expression in (6) is positive. We note that the condition

$$2\omega=\delta_+ +\delta_-, \tag{8}$$

under which, according to (6), $\Omega''(k,Q)$ has nearly its maximal value, corresponds approximately to the condition of wave synchronization for a four-wave process. The latter describes the conversion of two quanta of the dominant wave into two satellite quanta.

Next, assuming that $0\leq k\leq\pi$, when the relative anharmonic frequency shift satisfies the condition $\gamma=\tilde{K}_4/K_2\ll 1$, from (7) and (8) we obtain the following equations for Q

$$\cos(Q/2)=(1-\gamma)\quad\text{for } k>Q, \tag{9}$$

$$\sin(Q/2)=(1-\gamma)\tan(k/2)\quad\text{for } k<Q,\ k+Q<2\pi. \tag{10}$$

The other two combinations of signs from expanding the absolute value in (8) do not give new solutions.

The solution of Eq. (9) exists only under the condition $\gamma>0$ and has the approximate form $Q_m\approx\sqrt{8\gamma}$, while Eq. (10) has solutions for any sign of γ in the range $k_0\leq k<\pi/2+\gamma$. Here $k_0=0$ holds for $\gamma<0$, and $k_0\approx\sqrt{8\gamma}$ for $\gamma>0$, i.e., k_0 increases with increasing γ, narrowing the region of instability. Thus, just from an analysis of the condition (8) holds we arrive at several important conclusions: 1) when $K_4>0$, modulation instability is realized for all values of k, there being two independent regions of modulation instability in the space of Q for $k_0\leq k\pi/2+\gamma$; 2) at values of the wave vector of the carrier wave $k\leq\pi/2+\gamma$ modulation instability is realized for nonlinearity of either sign; 3) when $K_4<0$ holds the traveling wave breaks up mainly by generating waves propagating in the opposite direction.

3. RESULTS OF THE NUMERICAL EXPERIMENT AND DISCUSSION

Let us now move on to a discussion of the results of the numerical experiment simulating the dynamics of the anharmonic lattice (1). A standard conservative difference scheme was used in the simulation to numerically solve the system of equations of motion. A carrier traveling wave $A_0\cos[kn-\omega(k)t]$ and a perturbative wave

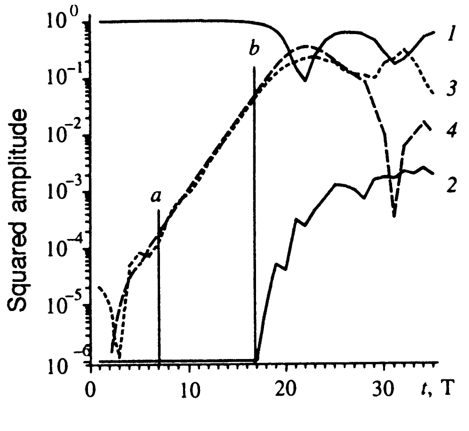

FIG. 1. Behavior of the squares of the amplitudes of a carrier wave with $k=3\pi/4$ (*1*), a third harmonic (2), and satellites of the carrier wave having the wave vectors $k\pm Q$ with $Q=14\pi/128$ (*3* and *4*, respectively). The segment *ab* corresponds to an exponential increase in the amplitude of the satellites.

$0.005A_0\cos[(k-Q)n-\omega(k-Q)t]$ were excited to investigate modulational instability in a lattice consisting of 256 particles. After a time on the order of several oscillation periods of the carrier wave $2\pi/\omega$, a satellite with a wave vector $k+Q$ formed, and the period of exponential increase in the amplitudes of both satellites began (curves *3* and *4* in Fig. 1). The growth rate $\Omega''(k,Q)$ was determined in just this period (segment *ab* in Fig. 1). We note that the influence of the third harmonic (curve *2* in the figure) can, in fact, be disregarded in the case under consideration, since its amplitude is negligibly small.

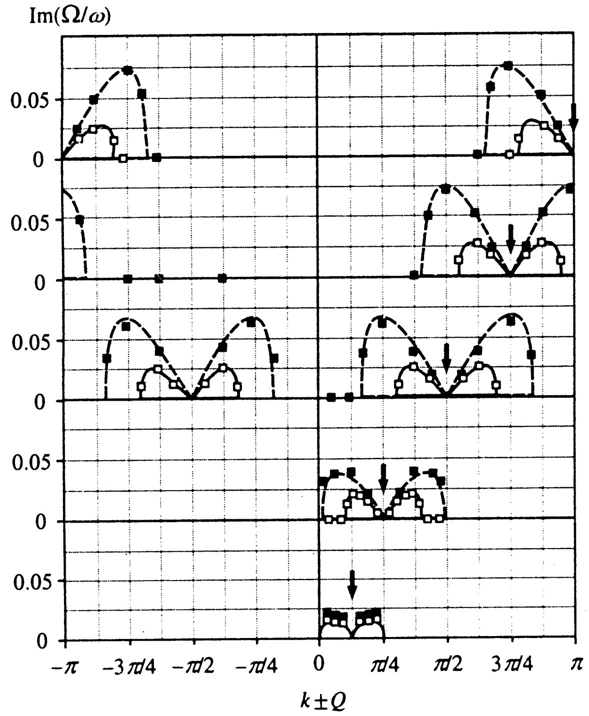

FIG. 2. The growth rate $\Omega''(k,Q)/\omega$ as a function of the wave vector of the perturbative wave $k\pm Q$ for various values of the wave vector k of the carrier wave (the values of k are indicated by the arrows). Solid lines – calculation based on Eq. (5) for $\gamma=0.03$; dashed lines – calculation for $\gamma=0.1$; unfilled squares – results of the numerical experiment for $\gamma=0.03$; filled squares – results for $\gamma=0.1$.

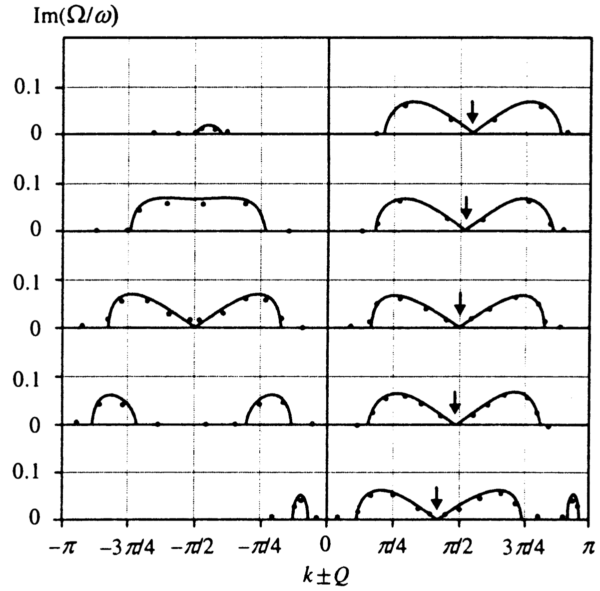

FIG. 3. The growth rate $\Omega''(k,Q)/\omega$ for wave vectors of the carrier wave (their values are indicated by the arrows) in the vicinity of $\pi/2$. Curves – calculation based on Eq. (5) for $\gamma=0.1$; points – results of the numerical experiment.

Figure 2 shows the dependence of the growth rate $\Omega''(k,Q)$ for two values of γ and various values of k. For $k=\pi$ and $3\pi/4$ reversal of the instability region of the satellite with the wave vector $k+Q$ can be seen. For $k=\pi/4$ and $\pi/8$ modulation instability is realized mainly for perturbative waves propagating in the same direction as the carrier wave. In the vicinity of $k\approx\pi/2$ the two instability regions mentioned above are observed, and they become identical at $k=\pi/2$. The transformation of the instability regions as the wave vector of the carrier wave varies near $\pi/2$ is shown in Fig. 3. As is seen from Figs. 2 and 3, the theoretical curves accurately describe the results of the numerical experiment over almost the entire range of values of k. The deviations observed for $\gamma=0.1$ and $k\leqslant\pi/8$ are caused by the influence of the generation of the third harmonic, which was not taken into account in our analysis. This influence cannot be neglected in the region of small carrier wave vectors, where the dispersion of the frequency is nearly linear. In particular, the generation of harmonics makes a definite contribution to the exchange of energy between the lowest modes of the FPU lattice.

The transformation of the modulational-instability regions for $K_4<0$ is depicted in Fig. 4. As is seen from the figure, in this case only the "additional" instability region remains, and qualitative agreement between the numerical experiment and the theoretical analysis is also observed as a whole.

The results of the numerical investigation of the dynamics of the system at times greatly exceeding the period of

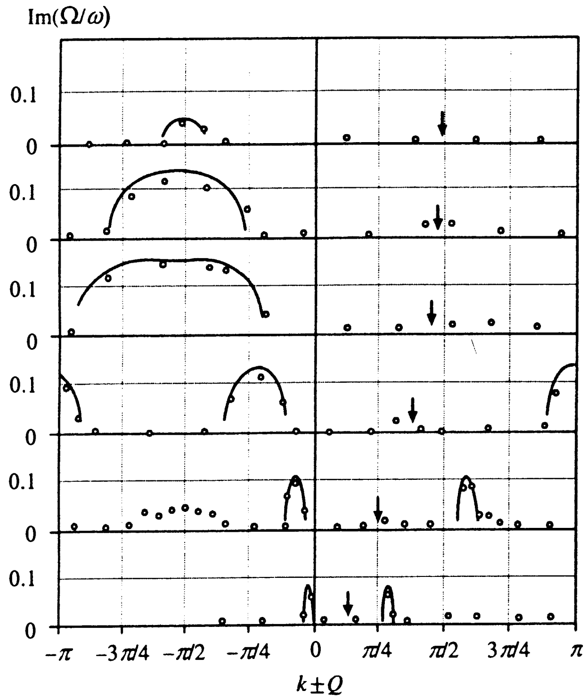

FIG. 4. The growth rate $\Omega''(k,Q)/\omega$ for wave vectors of the carrier wave (their values are indicated by the arrows) in the vicinity of $\pi/2$. Curves – calculation based on Eq. (5) for $\gamma=-0.1$; points – results of the numerical experiment.

exponential decay of the carrier wave is shown in Fig. 5 for $k=3\pi/4$ and $Q=\pi/8$. In analogy to the modulational instability of traveling waves in a continuum nonlinear system, an FPU lattice also displays recurrence phenomena controlled by the modulational instability, which are destroyed due to the generation of additional perturbative waves in the modulational-instability region as a result of the unavoidable inaccuracies in the numerical integration of Eqs. (1). Before proceeding to a discussion of the numerical results obtained, we note that there have been significant achievements in the analytical description of the long-term evolution of various periodic initial conditions in the case of continuum systems described by the nonlinear Schrödinger equation.[15,16] We note that methods using finite-band potentials, which give solutions in a form that is fairly difficult to analyze and is applicable only to fully integrable systems, was not used in those studies. For example, in Ref. 15 a periodic solution was obtained on the basis of a three-mode model, and the corresponding recurrence period, which agreed well with the results of the numerical experiment, was calculated. In Ref. 16 an exact periodic solution of the nonlinear Schrödinger equation which takes into account the influence of higher perturbative harmonics was constructed for the case in which the perturbative harmonics fall in the modulational-instability region of the carrier wave. Similar solutions have not yet been obtained for discrete systems, particularly for FPU lattices.

One significant difference between an FPU lattice and a continuum system is that the recurrence pattern shown in Fig. 5 changes drastically when k and/or Q are varied even by as little as $\pi/128$. This is clearly seen in Fig. 6, which depicts the evolution of a system having a carrier wave with $k=(3/4+1/128)\pi$ and a perturbative wave with $Q=\pi/8$ excited at the onset. As follows from Figs. 5 and 6, up to a time $120T$ ($T=2\pi/\omega$), which amounts to about three recurrence periods, the pictures of the evolution of the system in the two cases coincide. However, in the latter case (Fig. 6) the recurrence process is subsequently disrupted and an irreversible outflow of energy from the dominant mode begins, while in the former case (Fig. 5) the recurrence pattern is maintained up to times equal to $200T$. Finally, at times greater than $200T$ the energy in both cases is irreversibly redistributed among lattice modes which belong mainly to the instability

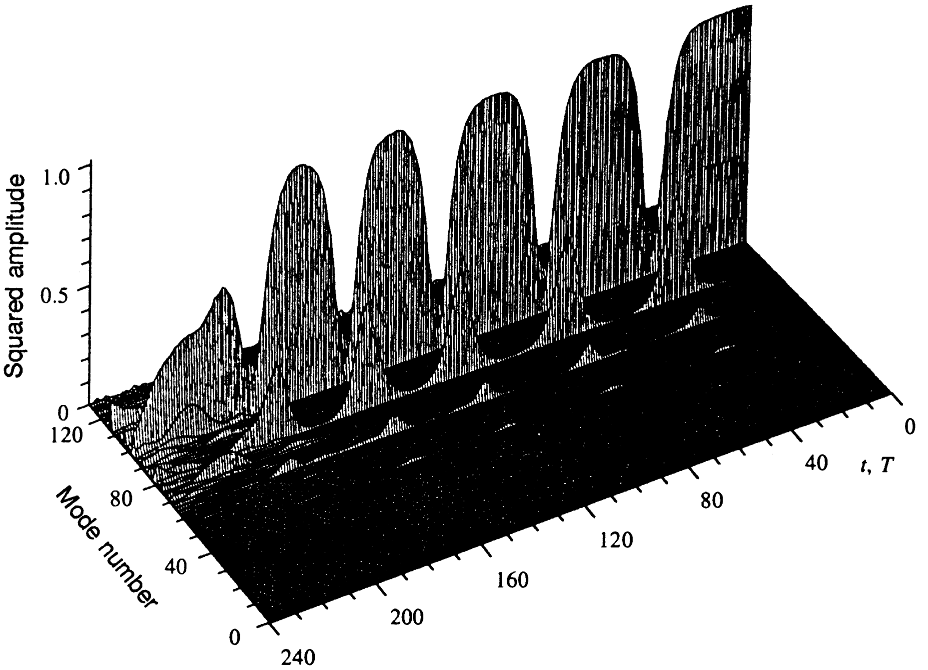

FIG. 5. Evolution of waves in an FPU lattice. A carrier wave with $k=3\pi/4$ (mode number 96) and $\gamma=0.03$ and a weak perturbative wave with $Q=\pi/8$ (mode number 80) were excited at the onset.

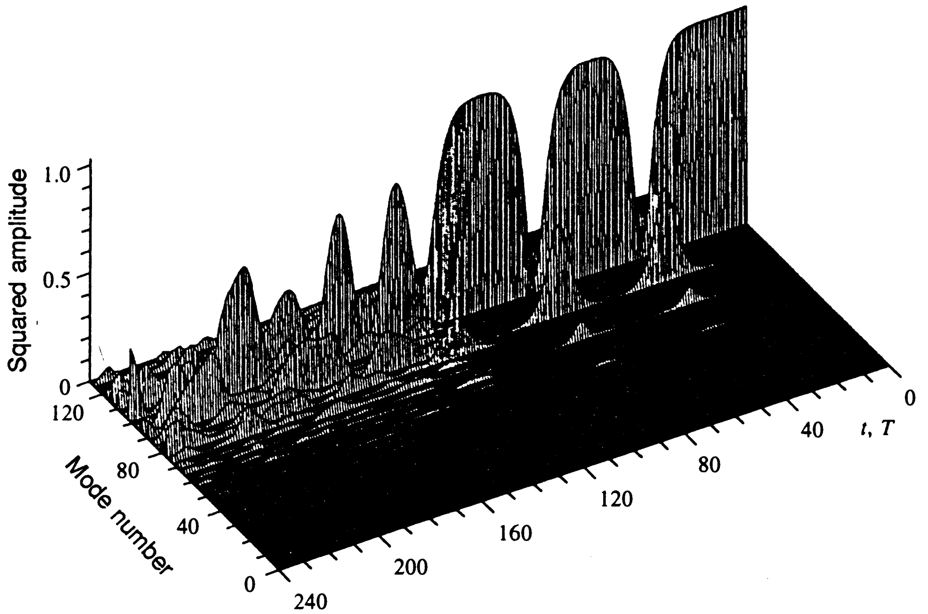

FIG. 6. Evolution of waves in an FPU lattice. A carrier wave with $k=(3/4+1/128)\pi$ (mode number 97) and $\gamma=0.03$ and a weak perturbative wave with $Q=\pi/8$ (mode number 81) were excited at the onset.

zone of the dominant wave. The observed strong dependence of the temporal evolution of the system on the initial conditions clearly reflects the discrete nature of the lattice and is specified by differences in the processes of induced (i.e., not associated with the inaccuracy of the numerical calculation) excitation of the additional perturbative waves in the modulational-instability region of the dominant wave. One possible mechanism for generating these perturbative waves is the reversal of any weak combination tone, for example, the third harmonic of the $k+Q$ mode, the ninth harmonic of the dominant wave, etc., in the first Brillouin zone. Thus, in the former case the third spatial harmonic of the $k+Q$ mode coincides with the $k-Q$ mode, while in the latter case it excites the additional unstable $k-Q+\pi/64$ perturbative wave, thereby accelerating the process of the disruption of recurrence phenomena. A more detailed discussion of this question requires additional research.

The numerical analysis also shows that even in a fairly early stage of the evolution of the system, the main process of energy transfer between the carrier wave and the perturbative waves is accompanied by the excitation of higher perturbative harmonics, i.e., $k\pm nQ$ modes. The excitation of the nth mode is a consequence of the instability of the $(n-1)$th mode toward the four-wave process of its breakup into two neighboring harmonics. For example, at times equal to $40T$, when the $k-Q$ mode has accumulated sufficient energy, it begins to break up into two satellites with the wave numbers k and $k-2Q$, the role of the seed wave being played by the k mode.

4. CONCLUSIONS

The investigations performed in the present work revealed several features of the modulational instability of traveling waves in Fermi–Pasta–Ulam lattices. The most important feature is the fact that these lattices have additional modulational-instability regions, which are not observed in the continuum models and correspond to the generation of perturbative waves propagating in the opposite direction, regardless of the sign of the quartic nonlinearity. These features of the modulational instability in an FPU lattice also differ significantly from those discovered in Ref. 9 for a Klein–Gordon lattice, which has only the single modulational-instability region characteristic of continuum systems and only for part of the Brillouin zone of the wave vectors of the carrier wave. We note, however, that the results in Ref. 9 were obtained in the approximation of weak dispersion of the oscillation frequencies. It can be shown that if the width of the band of optical modes is not small compared with the frequency $\omega(k=0)$, the structure of the modulational-instability regions and their restructuring as a function of the wave vector of the carrier wave are qualitatively similar to those discovered above. Thus, it is hoped that the appearance of additional modulational-instability regions corresponding to the generation of perturbative waves propagating in the reverse direction is a universal feature of the modulational instability of traveling waves in discrete systems with quartic nonlinearity of either sign.

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