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Spectrum of nonlinear excitations of modulated nanoclusters

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The nonlinear dynamics of a chain of four coupled anharmonic oscillators with alternating frequency parameters is investigated. This system is treated as an elementary fragment of a discrete modulated nonlinear medium, in particular, a medium of magnetic and elastic nanoclusters and coupled optical waveguides. The stationary monochromatic oscillations of the system are investigated analytically and numerically, and a complete classification of them is carried out. The bifurcation diagram for such a system is obtained: the spectral dependences of the oscillation frequencies on the integral of the number of states are found. A detailed investigation of the bifurcation process for the appearance of an excitation which is an analog of the gap soliton in a finite-size modulated medium is carried out. [DOI: 10.1063/1.2001645]

1. INTRODUCTION

Recently a great deal of attention in condensed matter physics is being devoted to the study of nonlinear self-localized excitations. Their fundamental role in the description of nonlinear phenomena follows directly from the results of the mathematical theory of solitons. This theory treats solitons and breathers as a qualitatively new basis of fundamental nonlinear excitations.[1,2]

However, in real microscopic media, when such physical factors as the discreteness and finite size of the system and dispersion and dissipation are taken into account, the properties of such nonlinear excitations can be altered significantly. This has been confirmed by the results of intensive numerical investigations of the nonlinear dynamics of discrete systems with a complex internal structure.[3–5]

The difficulties of the analytical description of the properties of nonlinear excitations in essentially discrete systems are due to the fact that the number of integrable models in this case is extremely small. It is well known that in the approximation of weak nonlinearity the problem of nonlinear localization for a wide range of applications can be discussed in the framework of the nonintegrable discrete nonlinear Schrödinger equation (DNSE).[4,6] Such an equation arises, e.g., in the description of nonlinear properties of a superlattice—in models of photonic and phononic crystals.[7,8] It is straightforward to show that solitons of the breather type in systems with distributed parameters have analogs in the DNSE system with two degrees of freedom. Thus the physical cause of the localization of excitations in nonlinear systems, i.e., the existence of solitons, can be understood from consideration of an extremely simple model of two coupled anharmonic oscillators.[9,10] For interpretation of more-complex objects and phenomena of nonlinear dynamics one must consider finite-size dynamical systems with a large number of degrees of freedom.[2,11]

Such a situation arises in systems with a complex internal structure, in particular, in finite-size modulated media. Examples of such systems are diatomic atom clusters on the surface of a crystal[12] and alternating superstructures—fragments of complex superlattices of photonic and phononic crystals. Such two-dimensional models arise in nonlinear optics, where they correspond to finite sets of nonlinear waveguides with alternating values of the frequency parameters.[8] Among electronic systems examples of one-dimensional objects with alternating charge structure that admit the existence of solitons and quantum breathers are MX chains.[13]

In low-temperature physics magnetic molecular nanoclusters are examples of finite-size modulated systems.[14–16] The total number of spins in such systems is small. A typical example of a magnetic molecule closed into a ring is the compound Mn_6R_6 (Ref. 16), in which the magnetic ions Mn with spin 5/2 alternate with ions of the radicals R having spin 1/2. Transitions in a magnetic field between states of the magnetic molecule with different values of the total spin are essentially quantum phenomena. However, the basic properties of the linear oscillation spectra of magnetic molecules and their weakly nonlinear oscillations about the ground state can be treated in the framework of the classical finite-size modulated DNSE model with a subsequent quasi-classical quantization of the spectrum of those oscillations.

A feature of the spectrum of linear excitations of a modulated system is the presence of a frequency gap in which linear oscillations are forbidden. In a nonlinear modulated medium the existence of so-called gap solitons, with frequencies lying in the gap of the spectrum of linear waves, is possible. The existence of gap (Bragg) solitons was first predicted theoretically in Refs. 17 and 18 in a study of the propagation of nonlinear waves in optical media with a modulated index of refraction. The simplest crystal structure that admits the existence of gap solitons is a diatomic chain with alternating masses of the atoms.[19–21] Since in the case of modulated nonlinear structures there are practically no integrable models, the first order of business is to study the simplest finite-size fragments of these systems which reflect the basic properties of modulated media, their qualitative analysis, and the numerical simulation of their dynamics.

In the present article, for the purpose of understanding the nature of the gap solitons and the causes of their formation and transformation with changing frequency we study the dynamics of a fragment of an anharmonic diatomic chain of four particles in the framework of the DNSE model. In such a system it is quite simple to investigate the monochromatic oscillations corresponding to stationary states of the nonlinear system and to carry out a complete classification of them, in particular, to find analogs of the gap and "out-of-gap" solitons. We obtain the quasi-classical spectra of nonlinear single-frequency oscillations, and we investigate in detail the bifurcation mechanism of formation of the analog of a gap soliton and the features of its transformation to an analog of the out-of-gap soliton at the lower boundary of the gap of linear excitations.

2. FORMULATION OF THE MODEL

We consider a system of four coupled anharmonic oscillations with alternating frequency parameters. For simplicity we assume cyclic boundary conditions, i.e., we close the chain into a ring. The Hamiltonian of such an extremely simple modulated system can be written in the form:

$$\mathcal{H}=\sum_{i=1}^{4}\left\{\tilde{\omega}_0^{(i)}|\psi_i|^2-\frac{1}{2}|\psi_i|^4+\varepsilon|\psi_i-\psi_{i-1}|^2\right\}, \tag{1}$$

where $\psi_0=\psi_4$ and $\tilde{\omega}_0^{(1)}=\tilde{\omega}_0^{(3)}$, $\tilde{\omega}_0^{(2)}=\tilde{\omega}_0^{(4)}$. Such a system describes, for example, an "elementary" fragment of a magnetic molecule of four spins with easy-axis anisotropy. Here the complex functions ψ_i are related to the components of the spin as follows: $\psi_i=S_i^x+iS_i^y$. The parameters $\tilde{\omega}_0^{(1,2)}$ correspond to the eigenfrequencies of the linear oscillations of two sorts of oscillators, and the constant ε characterizes the interaction of the particles with each other.

The dynamical equations corresponding to Hamiltonian (1) for these oscillations have the form

$$i\dot{\psi}_i-\omega_0^{(i)}\psi_i+|\psi_i|^2\psi_i+\varepsilon(\psi_{i+1}+\psi_{i-1})=0, \tag{2}$$

where we have introduced the notation $\omega_0^{(i)}=\tilde{\omega}_0^{(i)}+2\varepsilon$.

We note that Eq. (2) has an additional integral of motion besides an the total energy E of the system, viz., the number of quasiclassical states:

$$N=\sum_{i=1}^{4}|\psi_i|^2. \tag{3}$$

This quantity corresponds to an adiabatic invariant of the system and in the case of quasi-classical quantization it determines the number of quantum states with energies less than E.

The system of Eq. (2) has monochromatic solutions of the form

$$\psi_i=\varphi_i\exp(-i\omega t), \quad i=1,2,3,4, \tag{4}$$

which describe nonlinear stationary oscillations characterized by a single parameter—the frequency ω. We consider only real amplitudes φ_i. After substitution of expression (4) into system (2) we obtain a system of nonlinear algebraic equations

$$(\omega-\omega_0^{(i)})\varphi_i+\varphi_i^3+\varepsilon(\varphi_{i+1}+\varphi_{i-1})=0. \tag{5}$$

The difference of the frequencies of the oscillations is characterized by the parameter $\gamma=\omega_0^{(2)}/\omega_0^{(1)}$. Below we shall denote $\omega_0^{(1)}$ as ω_0 and $\omega_0^{(2)}=\gamma\omega_0$, and without loss of generality we can set the parameter ε equal to unity. For definiteness we shall assume $\gamma\geq 1$. The limit $\gamma\to 1$ corresponds to a uniform chain. For the case of a uniform chain ($\gamma=1$) the corresponding problem of monochromatic oscillations was formulated and solved completely in Ref. 5.

In the linear limit the spectrum of eigenfrequencies of the system consists of four values corresponding to in-phase oscillations with frequency $\omega_1=\Omega_+-\sqrt{\Omega_-^2+4}$, where $\Omega_\pm=\omega_0(1\pm\gamma)/2$, antiphase oscillations with frequency $\omega_4=\Omega_++\sqrt{\Omega_-^2+4}$, and two antiphase oscillations in each of the "sublattices," with frequencies $\omega_2=\omega_0^{(1)}$ and $\omega_3=\omega_0^{(2)}$. These oscillations correspond to the standard notation ($\uparrow\uparrow\uparrow\uparrow$), ($\uparrow\downarrow\uparrow\downarrow$), ($\uparrow 0 \downarrow 0$), and ($0\uparrow 0\downarrow$). The length and direction of the arrows characterize the relative amplitude and phase of the oscillations of the particle. The zeros correspond to nonmoving particles.

With increasing number of particles in the chain the number of frequencies in the spectrum will grow, and the new frequencies will occupy the frequency intervals (ω_1,ω_2) and (ω_3,ω_4). Here two zones of the spectrum are formed, with a gap between frequencies ω_2 and ω_3. Thus the values of the frequencies ω_2 and ω_3 play the role of the boundaries of a gap in the spectrum of linear excitations.

In the nonlinear case the frequencies of monochromatic oscillations depend on the amplitude and, hence, on the energy of the system and the number-of-states integral N: $\omega_i=\omega_i(N)$. For nonlinear oscillations it would be natural to use as the spectral characteristic the dependence of the total energy on the integral N: $E=E(N)$, which is in fact the quasi-classical spectrum of the system. It is not hard to show that for single-frequency solutions the important relation $\omega=dE/dN$ is satisfied. Therefore, in this paper we consider the spectral density $\omega=\omega(N)$ for a given oscillation, which also uniquely determines the dependence $E=E(N)$, as the basic characteristic of the nonlinear oscillations.

3. ANALYTICAL RESULTS

The initial system of nonlinear Eq. (2) cannot be integrated completely, since for the given problem the criterion of integrability is not met (the number of independent integrals is only equal to half of the total number of equations). Nevertheless, the system of algebraic Eq. (5) admits a substantial reduction to the two-particle problem. As a result, certain solutions, in particular the principal nonlinear oscillations corresponding to the boundaries of the "nonlinear" gap can be found exactly.

Indeed, by adding and subtracting equations of the system (5) in pairs for the 1st and 3rd and 2nd and 4th particles, changing to the new variables $\varphi_1-\varphi_3=u$, $\varphi_1+\varphi_3=\nu$, $\varphi_2-\varphi_4=x$, and $\varphi_2+\varphi_4=z$, and introducing the notation $A=\omega_0-\omega$ and $B=\gamma\omega_0-\omega$, we obtain a system of nonlinear algebraic equations for the differences and sums of the amplitudes of the oscillations of the oscillators:

$$
\begin{aligned}
&u[4A-(3\nu^2+u^2)]=0,\\
&x[4B-(3z^2+x^2)]=0,\\
&\nu[4A-(3u^2+\nu^2)]-8z=0,\\
&z(4B-(3x^2+z^2))-8\nu=0.
\end{aligned}
\tag{6}
$$

The system of Eqs. (6) clearly decomposes into four independent systems of equations:

Case (I): $u=0$, $x=0$,

$$\nu(4A-\nu^2)-8z=0,\quad z(4B-z^2)-8\nu=0. \tag{7}$$

Case (II): $u=0$, $x^2=4B-3z^2$,

$$\nu(4A-\nu^2)-8z=0,\quad z(z^2-B)-\nu=0. \tag{8}$$

Case (III): $x=0$, $u^2=4A-3\nu^2$,

$$z(4B-z^2)-8\nu=0,\quad \nu(\nu^2-A)-z=0. \tag{9}$$

Case (IV): $u^2=4A-3\nu^2$, $x^2=4B-3z^2$,

$$z(z^2-B)-\nu=0,\quad \nu(\nu^2-A)-z=0. \tag{10}$$

Thus the initial problem for four particles actually reduces to four independent problems for two coupled nonlinear oscillators, and the whole frequency spectrum for the amplitudes of nonlinear monochromatic oscillations of the system (5) is composed of four sets of spectral curves $\omega_i=\omega_i(N)$, corresponding to the cases (I)–(IV). We note that the system of equations for the amplitudes ν and z in the general case can have up to 9 real solutions (one trivial solution $\nu=z=0$ and four pairs of solutions differing only in sign). This permits the assertion that in the stated problem for a given type of monochromatic oscillations there are 19 nontrivial spectral curves $\omega_i(N)$.

The principal nonlinear oscillations of the system are in-phase and antiphase oscillations and also oscillations corresponding to the boundaries of the "nonlinear" gap of the spectrum. For the in-phase and antiphase nonlinear oscillations $\varphi_1=\varphi_3$ and $\varphi_2=\varphi_4$, and the problem of finding the corresponding solutions therefore requires consideration of case (I).

Using the connection between the amplitudes of the oscillations and the integral $N\equiv n/2=(\nu^2+z^2)/2$, one can obtain expressions for ν^2 and z^2:

$$\nu^2=\frac{n(\beta-n)}{\alpha+\beta-2n},\quad z^2=\frac{n(\alpha-n)}{\alpha+\beta-2n},$$

where $\alpha=4A$, $\beta=4B$. Substituting the expressions obtained into the equation $(A-\nu^2)(B-z^2)=64$, which follows from system (7), we arrive at a fourth-order equation for n:

$$n^4-3Cn^3+Dn^2-Fn+G=0. \tag{11}$$

Here we have introduced the notation $C=\alpha+\beta$, $D=\alpha\beta+3C^2-256$, $F=C(2\alpha\beta+C^2-256)$, $G=C^2(\alpha\beta-64)$.

The roots of Eq. (11) are the functions $n(\omega)$, which can be inverted to give the functions $\omega_i(N)$ and, most importantly, the spectral curves corresponding to the in-phase and antiphase oscillations of the particles.

Case (II) contains the exact solution $\nu=z=0$ corresponding to the upper boundary of the "nonlinear" gap $(0\uparrow 0\downarrow)$, which in terms of the amplitudes of the oscillations of the oscillators has the form $(0,\sqrt{B},0,-\sqrt{B})$. The spectral dependence for this boundary of the gap is easily found in explicit form: $\omega_3(N)=\gamma\omega_0-N/2$.

The exact solution corresponding to the lower boundary of the gap $(\uparrow 0\downarrow 0)$ is contained in case (III) and has the form $(\sqrt{A},0,-\sqrt{A},0)$. This corresponds to the spectral dependence $\omega_2(N)=\omega_0-N/2$.

In case (IV) there is yet another exact solution, corresponding to an oscillation of the type $(\uparrow\uparrow\downarrow\downarrow)$. The amplitudes of the oscillations of the particles for this solution are equal to $(\sqrt{A},\sqrt{B},-\sqrt{A},-\sqrt{B})$. The spectral density corresponding to this solution is also obtained in explicit form: $\omega_b(N)=\omega_0(1+\gamma)/2-N/4$. It is split off in the manner of a bifurcation from the upper boundary of the gap at a frequency $\omega_*=\omega_0$.

Moreover, it can be shown that all of the points of the bifurcations from the branches of the boundary of the "nonlinear" gap can be found exactly. For this we write solutions close to the solution $(0,\sqrt{B},0,-\sqrt{B})$ in the following form: $\varphi_1=\psi_1$, $\varphi_2=\sqrt{B}+\psi_2$, $\varphi_3=\psi_3$, $\varphi_4=-\sqrt{B}+\psi_4$, where $\psi_i<1$. Substituting the expressions for the functions φ_1, φ_2, φ_3, and φ_4 into the initial system of Eq. (5), we obtain the following linearized system for the small corrections ψ_i:

$$
\begin{aligned}
&(\omega-\omega_0)\psi_1+(\psi_2+\psi_4)=0,\\
&2(\gamma\omega_0-\omega)\psi_2+(\psi_1+\psi_3)=0,\\
&(\omega-\omega_0)\psi_3+(\psi_2+\psi_4)=0,\\
&2(\gamma\omega_0-\omega)\psi_4+(\psi_1+\psi_3)=0.
\end{aligned}
\tag{12}
$$

Equating the determinant of the matrix of coefficients of the system (12) to zero, we arrive at an equation for the bifurcation frequencies:

$$(\gamma\omega_0-\omega)(\omega_0-\omega)[(\omega-\omega_0)(\gamma\omega_0-\omega)-2]=0. \tag{13}$$

The solution $\omega=\gamma\omega_0$ is trivial. The solution with $\omega_*=\omega_0$, as we have said, corresponds to the splitting off of the exact solution $(\sqrt{A},\sqrt{B},-\sqrt{A},-\sqrt{B})$. Finally, the two roots

$$\omega_{1,2}=\frac{1}{2}\left(\omega_0(1+\gamma)\pm\sqrt{\omega_0^2(1-\gamma)^2-8}\right) \tag{14}$$

arise only above a certain critical value $\gamma_c=1+2\sqrt{2}/\omega_0$. As an analysis shows, the spectral curves $\omega_i(N)$ corresponding to these two bifurcation solutions behave in an extremely nontrivial way with increasing N. One of these curves goes into the region of the nonlinear gap, while the other splits off as an ordinary bifurcation but then, with increasing N, both functions lie outside the gap and terminate at their intersection point at a certain value N_c. When the parameter γ reaches a threshold value γ_* this point becomes a quadracritical point (at which four solutions come together), and from that point on there exist two infinite intersecting lines of the analog of the gap soliton and an ordinary primary

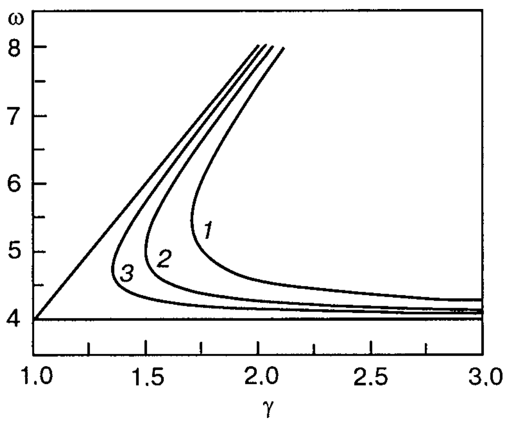

FIG. 1. Dependence of the bifurcation frequencies (upper branches of the hyperbolas) on the parameter γ for analogs of gap solitons in systems of coupled anharmonic oscillators of two sorts: for 4 particles—curve *1*; for 8 particles—curve *2*; for 12 particles—curve *3*.

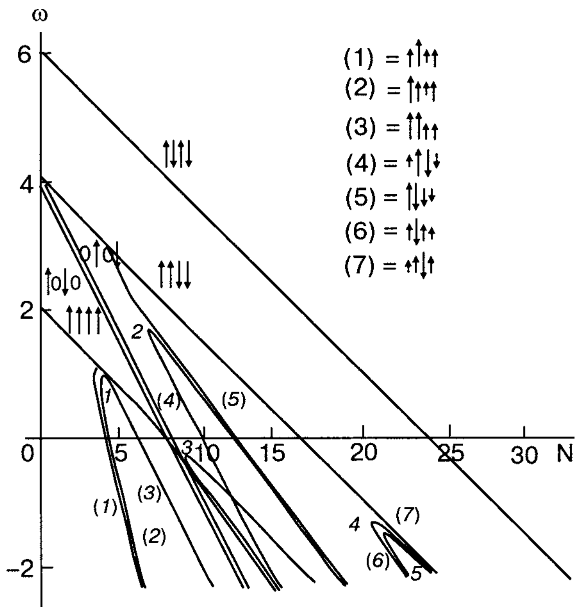

FIG. 2. Bifurcation diagram of single-frequency solutions for systems of four coupled anharmonic oscillators for $\gamma=1.025$.

bifurcation dependence split off from the upper boundary of the gap.

Thus, starting at the value $\gamma_*=1.750$ the upper boundary of hyperbola *1* in Fig. 1 corresponds to bifurcation points of the analog of the gap soliton, the spectral dependence of which with increasing γ occupies a larger and larger place in the gap region. It is interesting to note that all of the points of bifurcation from the upper boundary of the "nonlinear" gap for systems of 8, 12, 16 and any other multiple of four are found in explicit form. Figure 1 also gives the curves of the bifurcation frequencies for analogs of the gap solitons for the cases of 8 and 12 particles. It is seen that the critical and threshold values γ_c and γ_* fall off rather rapidly with increasing number of particles, and for an infinite system they go to zero.

In conclusion we note that since equations of the fourth order in ω are obtained for the bifurcation frequencies in the case of four particles, the spectral curves of the nonlinear oscillations can exhibit not more than four bifurcation points. One is readily convinced that bifurcations are absent on the lines of antiphase oscillations and on the lower boundary of the gap.

4. RESULTS OF A NUMERICAL CALCULATION

Since the system of nonlinear algebraic Eq. (5) obtained above cannot be completely solved analytically, numerical methods were used. The calculation was done using the Maple 8 software package. For a specified value of the parameter $\omega_0=4$, all of the real solutions of the system of Eqs. (7)–(10) were found and, hence, the solutions of system (5) for a fixed value of the parameter γ and arbitrary ω. As a result, for the given value of ω we obtained a set of solutions $\varphi_i^{(j)}$, where the index i enumerates particles and j enumerates solutions. For each jth solution of the system (5) at a specified value of the frequency the value of the number of states of the system (3), which is an integral of the motion, was calculated. Thus, the spectral characteristics of the system were obtained: the dependences of the oscillation frequencies ω on the integral N.

Numerical integration of the equations was done for a wide range of values of the parameter γ. The main results are shown in Figs. 2, 3, and 4 for $\gamma=1.025$, $\gamma=1.76$, and $\gamma=20$.

The features of the bifurcation pattern for the functions $\omega=\omega(N)$ in the case of a small difference of the eigenfrequencies of the particles (for $\gamma=1.025$) are presented in Fig. 2.

First of all we see that in the modulated chain the spectrum of linear excitations has a gap. The presence of particles of two different eigenfrequencies leads to lifting of the degeneracy for oscillations of the form ($\uparrow 0 \downarrow 0$). For γ close to unity the gap is narrow, but it widens rather rapidly with increasing γ. As we mentioned in the previous Section, the solution $(\sqrt{A},\sqrt{B},-\sqrt{A},-\sqrt{B})$ splits off from the upper boundary of the gap at small N at a frequency equal to ω_0. Another solution splits off from the solution formed for $N \approx 4$. Now, however, unlike the case of the uniform chain, a subsequent bifurcation does not arise on the line of the new solution, and a lifting of the degeneracy occurs with the appearance of solutions (4) and (5), which form the "parabola" *2*. As will be seen later on, the position of this "parabola" varies rapidly with increasing γ.

In the case of a uniform chain a twofold degenerate dependence for oscillations with strong localization at one particle splits off in a bifurcation manner from the dependence for in-phase oscillations at a finite value of N. In the case of different particles this bifurcation splits and the degeneracy is lifted with the formation of solutions (1) and (2) (this is analogous to the lifting of the degeneracy in a system of two oscillators with different masses). Now a line *3*, which corresponds to an analog of the localized solution centered between particles in the uniform chain, splits off from line *2*. Yet another bifurcation point is found on the line of the in-phase oscillations at ω close to zero. Upon a small increase of the parameter γ a coalescence of this primary bifurcation and branch *2* occurs at a point $\gamma_*=1.05$, with the formation of "parabola" *1*. After the joining of the branches, "parabola" *1* begins to shift into the region of the nonlinear gap.

To describe the order of the positions of the spectral curves in the vicinity of $N=10$, $\omega\approx-1$, let us fix the value of the frequency and follow the appearance of the curves as N increases. The line of in-phase oscillations passes most closely to solution (3), and then come the lower and upper boundaries of the "nonlinear" gap. The left branch of the "parabola" *3* situated to the right of the line of the upper boundary of the gap and is inclined at the same angle to the N axis. Farther to the right, the primary bifurcation from the line of in-phase oscillations occurs, and next to it is a bifurcation formed on the left branch of "parabola" *3*.

Finally, we address the appearance of "parabolas" *4* and *5* as a result of the lifting of the degeneracy in the modulated chain. It is "parabola" *4* that with growth of the parameter γ takes part in the formation of the analog of the gap soliton.

As in an infinite modulated medium, an analog of the gap soliton in a chain with a small number of particles should correspond to a solution whose frequency lies in the region of the "nonlinear" gap. Such a solution actually arises with growth of the parameter γ, and this occurs in a threshold manner after the parameter γ reaches a critical value $\gamma_c=1.707$. We note that with increasing γ the relative size of the gap increases, and the main bifurcations on the line of in-phase oscillations and the upper boundary of the gap shift to smaller N. At the same time, the bifurcation "parabolas" *1* and *2* shift to the region of negative frequencies, penetrating into the gap region, and the sharp apex of "parabola" *4* approaches the upper boundary of the gap as the critical value γ_c is approached. The bifurcation diagram of above-threshold values of the parameter γ and in the immediate vicinity of γ_c is presented in Fig. 3 for $\gamma=1.76$. The inset shows the point of creation of the analog of the gap soliton. After the parameter γ reaches the critical value $\gamma_c=1.707$, two bifurcation points appear on the line of the upper boundary. The subsequent evolution of the solutions created at these bifurcation points occurs very specifically and in complete agreement with the description of this process in the previous Section for γ just less than the threshold value $\gamma_*=1.750$, having the form shown in the inset of Fig. 3. At a value $\gamma=1.76$ we see in Fig. 3 that instead of the sharp-ended "parabola" *4* there already exists a branch corresponding to the gap solution S and a branch of the ordinary primary bifurcation II. The first splits off and passes into the gap, then leaves the gap and crosses the horizontal axis at $N\approx18.7$. The second dependence splits off upward from the boundary of the gap and behaves as a typical primary bifurcation. We note that if we follow the change of γ, moving from the region of large values to the region of small values of this parameter, then the vanishing of the branch of gap solitons occurs at the moment when its bifurcation point approaches the point of the primary bifurcation and it culminates in the formation of a "parabola," which then moves out into the region of negative values.

Finally, we note that "parabolas" *3* and *5* no longer show up on the bifurcation diagram, since they move ever deeper into the region of negative frequencies.

With increasing γ the gap increases strongly, and the bifurcation point of the gap solution approaches the weakly nonlinear limit and corresponds to a frequency close to $\gamma\omega_0$. In this limit at small values of N there are two qualitatively very similar bifurcation patterns at low and high frequencies. This actually corresponds to the case of oscillations of atoms with substantially different masses, i.e., there are two almost independently oscillating systems of nonlinear oscillators with renormalized effective couplings. Both on the line of the upper boundary of the gap and on the line of the in-phase oscillations there are bifurcations of creation of quasi-soliton states by the scenario described by Ovchinnikov.[9] But the main effect, which becomes obvious in the limit of large γ, is the transformation of the analog of the gap soliton into an out-of-gap soliton. It occurs at a frequency close to the lower edge of the spectrum of linear oscillations, as can be seen on the bifurcation diagram in Fig. 4. The only lines that remain on it are those that fall into the region of the "nonlinear" gap and the curve for the oscillation $(\sqrt{A},\sqrt{B},-\sqrt{A},-\sqrt{B})$. The line of the analog of the gap soliton is split off from the

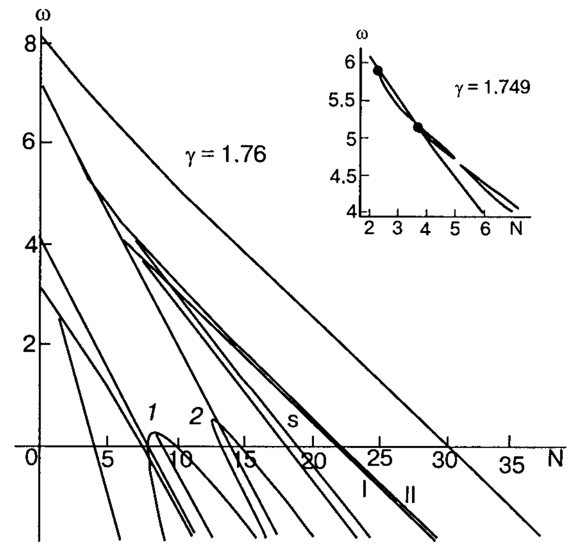

FIG. 3. Bifurcation diagram of single-frequency solutions for $\gamma=1.76$ (the inset shows the moment of creation of the analog of the gap soliton at a value just below the critical, $\gamma=1.749<\gamma_c=1.750$).

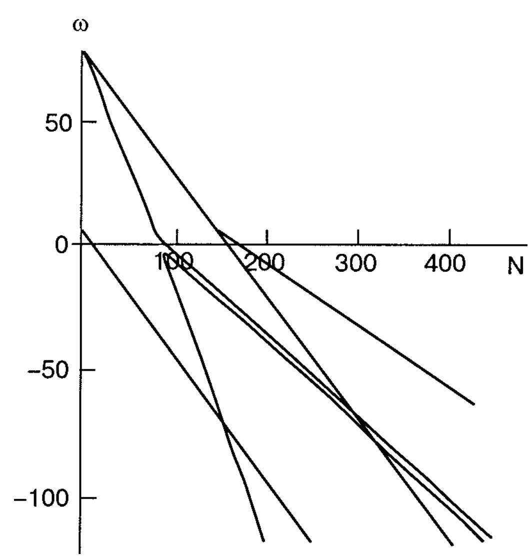

FIG. 4. Bifurcation diagram of single-frequency solutions at $\gamma=20$. The solution corresponding to the gap soliton is transformed into an out-of-gap soliton near the lower edge of the spectrum of linear waves.

upper boundary of the gap, reaches the frequency ω_0, and is continuously transformed into the line of the out-of-gap soliton. We recall that in an infinite system the out-of-gap soliton corresponds to localized oscillations of the atoms of one sort and nonlocalized oscillations of the atoms of the other sort. Anomalous changes of the relationships of the amplitudes are also traced in the finite-size system investigated here.

It should be stressed that in the case $\gamma \gg 1$ many of the characteristic features of the spectral curves of the system studied—simple and double primary bifurcations, secondary bifurcations, branching points, etc.—repeat the most essential elements of the dynamics of an anharmonic chain with a large number of degrees of freedom.[20] The appearance of a gap soliton and its transformation into an out-of-gap soliton in the investigated fragment of a modulated medium and in a system of large size occur according to an identical scenario. The presence of a larger number of degrees of freedom leads to filling of the regions below and above the ''nonlinear'' gap by frequency dependences, while the bifurcation pattern in the gap remains qualitatively the same.

From the standpoint of application of the results to magnetic molecules and systems of nonlinear optical waveguides with a small number of elements we note that the solutions found for four oscillators not only demonstrate the basic regularities of the formation of quasi-soliton states but are also part of the solutions for systems consisting of 8, 12, 16, etc., oscillators. It seems to us that it should be possible to excite quasi-soliton states (including gap solitons) by resonance methods in magnetic and elastic nanoclusters and optical waveguides. It should be kept in mind that the in-phase oscillations corresponding to quasi-soliton states and which are the discrete analogs of breathers in a finite-size system have the lowest energy for a fixed number of states. Indeed, the quasi-classical spectra of all the oscillations found are easily reproduced from the calculated dependences $\omega_i = \omega_i(N)$. Mainly these are originally quadratically growing functions that reach a maximum at points where the frequency goes to zero, after which they fall off with increasing amplitudes of the oscillations (with increasing integral N). However, it should be noted that, unlike the infinite and continuous systems of the nonlinear Schrödinger equation, the question of stability of the quasi-soliton states of the discrete nonlinear Schrödinger equation cannot be solved solely on the basis of an analysis of quasi-classical spectra, and it requires a special investigation.[22]

CONCLUSIONS

In summary, in a modulated finite-size nonlinear system the spectrum of single-frequency stationary states includes principal nonlinear oscillations and oscillations split off from the principal oscillations as a result of primary and secondary bifurcations, and also oscillations arising in pairs at finite values of the excitation energy (or integral N). The main results of our study of the stationary nonlinear oscillations of such a system can be summarized in the following statements.

1. We have obtained the complete bifurcation diagram of monochromatic solutions in a system of four oscillators and have carried out a general classification of their spectral curves $\omega_i = \omega_i(N)$ for an arbitrary relationship of the frequency characteristics of two sorts of oscillators.

2. We have described effects due to the modulated character of the system: the formation of a gap, the appearance of bifurcations and splitting (doubling) bifurcation curves, the formation of autonomous pairs of solutions which correspond to ''parabolic'' spectral curves, and also other features characteristic for systems with defects.

3. We have investigated in detail the process of formation of the solution that is the analog of the gap soliton in a distributed modulated medium. We have found the critical value γ_c (the critical ratio of eigenfrequencies of the oscillators) above which the gap solutions of the soliton type exist.

4. We have shown that at large gap sizes the existence region of such a solution is large; it arises in a bifurcation manner, similarly to the quasi-soliton state split off from the branch of uniform oscillations. At a value of the frequency close to the lower edge of the gap of linear oscillations, an analog of the gap soliton is transformed to an out-of-gap soliton. It is assumed that the quasi-soliton states, including the gap solitons, can be excited by resonance methods in magnetic and elastic nanoclusters and systems of optical waveguides.

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