Breathing self-localized solitons in the quartic Fermi-Pasta-Ulam chain

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If the fundamental self-localized soliton (SLS) of the Fermi-Pasta-Ulam chain is subjected to a perturbation of the same parity, a breathing behavior in space is observed. The time evolution then is characterized by two different frequencies. We show that the observed breathing behavior can be explained by means of a harmonic model with an effective spring hardening which is generated by the fundamental background SLS. The validity of this harmonic model is verified by means of numerical simulations. Improvements involving a parametric oscillator are mentioned but left to future study. [S0163-1829(96)00838-7]

I. INTRODUCTION

The existence of localized modes in a harmonic lattice containing point defects is well understood.[1] Recently, in the work of Dolgov[2] and of Sievers and Takeno[3] the existence of self-localized solitons (SLS) in anharmonic lattices without impurity was theoretically predicted. These SLS's are reminiscent of the defect-induced localized modes in the harmonic lattice and they can occur at any site of the anharmonic lattice. This was later confirmed by means of numerical simulations[4,5] and in recent works the properties of the SLS's have been further investigated.[6–11] In particular, it has been proved that the parity of the SLS's has a great relevance to their stability.[12,13]

In a previous investigation,[14,15] the present authors have investigated the generation of the SLS in the Fermi-Pasta-Ulam chain (FPU, see Refs. 16 and 17) with quartic anharmonicity by means of an external force acting on a single atom. The numerical simulations have shown the existence of a SLS with a spatial envelope characterized by a ''breathing'' behavior, where the spatial extension of the SLS changes periodically in time. We have denoted this localized mode ''breathing SLS'' and further numerical experiments have shown that this breathing behavior can persist for a very long time.

In this paper we investigate the properties of the breathing SLS's and we propose a harmonic model which explains the main features of these SLS's. The paper is organized as follows. In Sec. II we introduce the FPU model and in Sec. III we characterize the main properties of the SLS's in the quartic FPU chain. We then describe the numerical experiments and the features of the breathing SLS's (Sec. IV). In Sec. V we present a model for these breathing SLS's. Finally, in Secs. VI and VII we discuss the results obtained and present our conclusion.

II. THE FPU MODEL

We consider a regular one-dimensional chain (FPU chain) with nearest-neighbor harmonic and anharmonic interaction. The equation of motion for the displacement $Q_n(\tau)$ of the nth atom reads

$$\frac{d^2Q_n}{d\tau^2} = -\sum_{n'=n\pm 1} [(Q_n - Q_{n'}) + (Q_n - Q_{n'})^3], \tag{1}$$

where we have considered dimensionless variables (the coefficients of the linear and cubic terms can be set equal to one by means of a scaling transformation[11]). For the harmonic chain the maximal phonon frequency is indicated by Ω_D which we will denote as the Debye frequency and which is considered as a reference frequency ($\Omega_D = 2$). The Hamiltonian in our dimensionless variables is given by

$$H = \sum_n H_n = \sum_n \left\{ \frac{P_n^2}{2} + \frac{1}{4} \sum_{n'=n\pm 1} \left[(Q_n - Q_{n'})^2 + \frac{1}{2} (Q_n - Q_{n'})^4 \right] \right\}, \tag{2}$$

where $P_n = dQn/d\tau$ is the momentum of the nth atom and H_n is the dimensionless energy per lattice site.

III. SLS IN THE FPU CHAIN

The SLS's are vibrational modes with localization properties similar to those of a localized mode obtained in the harmonic chain with point defects. The main features of these SLS's are a frequency above the Debye frequency, antiphase elongations of neighboring atoms, and an exponential decrease of the wings. The SLS has a solution of monochromatic behavior and may be written in the approximate form

$$Q_n(\tau) = A_n(-1)^n \cos(\Omega\tau), \tag{3}$$

the overtones being of minor importance.

In the following we will express the maximal value of the amplitudes A_n of expression (3) by the variable A. Then we introduce the ''effective anharmonicity parameter'' $\gamma_4 = A^2$ which is a measure of the anharmonicity of the SLS. In fact, considering the equation of motion (1) we note directly that the importance of the cubic term increases in proportion to $\gamma_4 = A^2$.

For small values of $\gamma_4 (\gamma_4 \ll 1)$, the solutions involve a great number of particles, and in this limit the equations of motion (1) merge into a nonlinear Schrödinger equation in the continuum approximation of the lattice. This limit has been handled analytically by Yoshimura and Watanabe[8] and by Chubykalo *et al.*[13] They have found a solution, which in discrete notation may be written as

$$Q_n(\tau)=A(-1)^n \mathrm{sech}(\sqrt{6}An)\cos(\Omega\tau), \tag{4}$$

where the frequency Ω is given by $\Omega=\Omega_D+3/2A^2$.

On the other hand, for great effective anharmonicity ($\gamma_4 \gg 1$) the SLS is strongly localized, and practically only three or two particles, respectively, are involved. In this case approximate analytical solutions have been obtained by Sievers and Takeno[6] using lattice Green functions and the ''rotating wave'' approximation, whereby again only a single frequency is considered in the time dependence. The even-parity SLS ($Q_{n+1}=-Q_{-n}$) has a normalized displacement pattern[7] given approximately by $A(\ldots,0,-1,1,0,\ldots)$ and the correspondent odd-parity SLS ($Q_n=Q_{-n}$) has a pattern[6] given by $A(\ldots,0,-1/2,1,-1/2,0,\ldots)$ (the terms: ''odd'' and ''even'' refer to longitudinal types of motion). In this limit ($\gamma_4 \gg 1$) the displacement pattern is constant but the frequency of the SLS is proportional to γ_4.[9]

We mention also an alternative method (Gauss procedure) for the construction of rather accurate solutions proposed by two of the present authors.[11] This method can be applied for arbitrary values of the effective anharmonicity parameter γ_4. The method is based on an iterative Gaussian optimization and the knowledge of the limiting analytic form of the solution on the wing of the soliton. The solutions obtained with the Gauss procedure are in agreement with the previously cited solutions in both limits $\gamma_4 \gg 1$ and $\gamma_4 \ll 1$ and are accurate also in the intermediate regime. All these approximate solutions are monochromatic (i.e., only a single frequency is considered in the time dependence). However, one should be aware of the fact that the exact solutions contain always spectral components with odd multiples of the fundamental frequency Ω due to the presence of the anharmonic term in the equation of motion (1). These higher frequency components in the Fourier spectra have a small amplitude in comparison with the amplitude of the fundamental frequency[9] and are practically negligible.

IV. BREATHING SLS'S

In previous work[15,14] we have investigated the generation of solitons in the FPU chain by means of an external force acting for a restricted time period at a single site. It turned out that after sufficiently long time the amplitude of the vibrating atoms in the neighborhood of the excited site behaved in a ''breathing'' manner, which persisted for a very long time (''breathing SLS'').

To investigate this phenomenon more closely we now focus our attention on a more specific generation of the breathing solitons by choosing well-directed initial conditions. In our numerical experiments we evaluate the time evolution of the FPU chain by solving numerically the equation of motion (1) by a fourth-order Runge-Kutta method. The time step in our program is always chosen to preserve the total energy of the chain to an accuracy better than 10^{-5} and the lattice is treated in a self-expanding manner, which excludes the influence of the boundary conditions (for more detail on the numerical technique see Ref. 11). The initial condition for

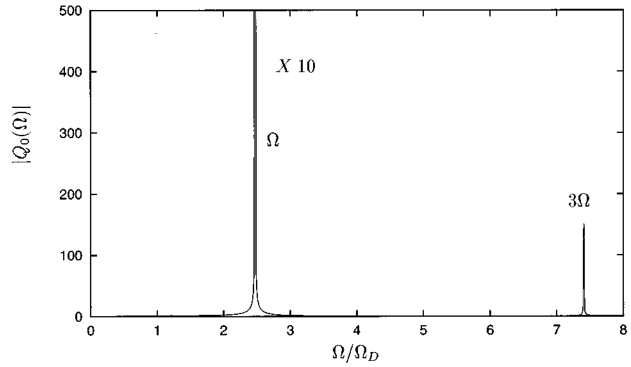

FIG. 1. Fourier transform of $Q_0(\tau)$ for an odd-parity SLS with $\gamma_4=4$ generated by the initial condition $Q_n(0)=2(\ldots,0,0.055,-0.54,1,-0.54,0.055,0,\ldots)$; $P_n(0)=0$. The peak with frequency Ω has an intensity 5×10^3 (arb. units).

our numerical simulations will be chosen to have a displacement pattern of the form

$$Q_n(0)=A_n(-1)^n; \quad P_n(0)=0 \tag{5}$$

We first choose the amplitudes A_n as they are found by the Gauss procedure introduced in an earlier paper.[11] In this case the initial condition very closely corresponds to a SLS, and the Fourier transform of the time evolution $Q_n(\tau)$ shows a single fundamental frequency. In Fig. 1 we show the Fourier transform of the displacement at the central site $n=0$ for the initial condition pertaining to an odd-parity SLS with $\gamma_4=4$. We note clearly the presence of only one fundamental frequency Ω and the overtone at 3Ω. The same result is obtained also if we chose initial conditions with even parity, and also for other values of γ_4. In the limit of small effective anharmonicity γ_4 the displacement pattern

$$A_n=A\ \mathrm{sech}(\mu n); \quad \mu=\sqrt{6}A \tag{6}$$

applies, as obtained from Eq. (4). This again constitutes a good initial condition and in the numerical simulation we observe only a fundamental frequency.

The appearance of other frequencies in the spectra of the displacements is found if we choose initial conditions different from the ''good'' initial conditions just described which almost correspond to an ''eigenmode'' of the FPU chain. For instance, if we consider a different ratio μ/A in the displacement pattern as that employed in Eq. (6), the resulting initial condition generates a breathing soliton which no longer is describable by expression (3). In Fig. 2(a) we show the time evolution of the displacement Q_0 at the center of the soliton obtained for an initial condition of the form Eq. (6) with a ratio $\mu/A=1$. We note that another frequency Ω_3 appears [see Fig. 2(b)] in the Fourier transform of the displacements. In Fig. 2(b) we show the Fourier transform for the central particle $n=0$. The other particles involved have a similar spectrum with unchanged positions of the peaks, although their relative intensity is altered. The modulation of the displacement [see Fig. 2(a)] is characterized by the difference frequency $\Omega-\Omega_3$, where Ω is the fundamental frequency of the SLS and Ω_3 is a new frequency generated by the ''perturbed'' initial condition. In this case the perturbation conserves the symmetry of the SLS, and the new frequency is

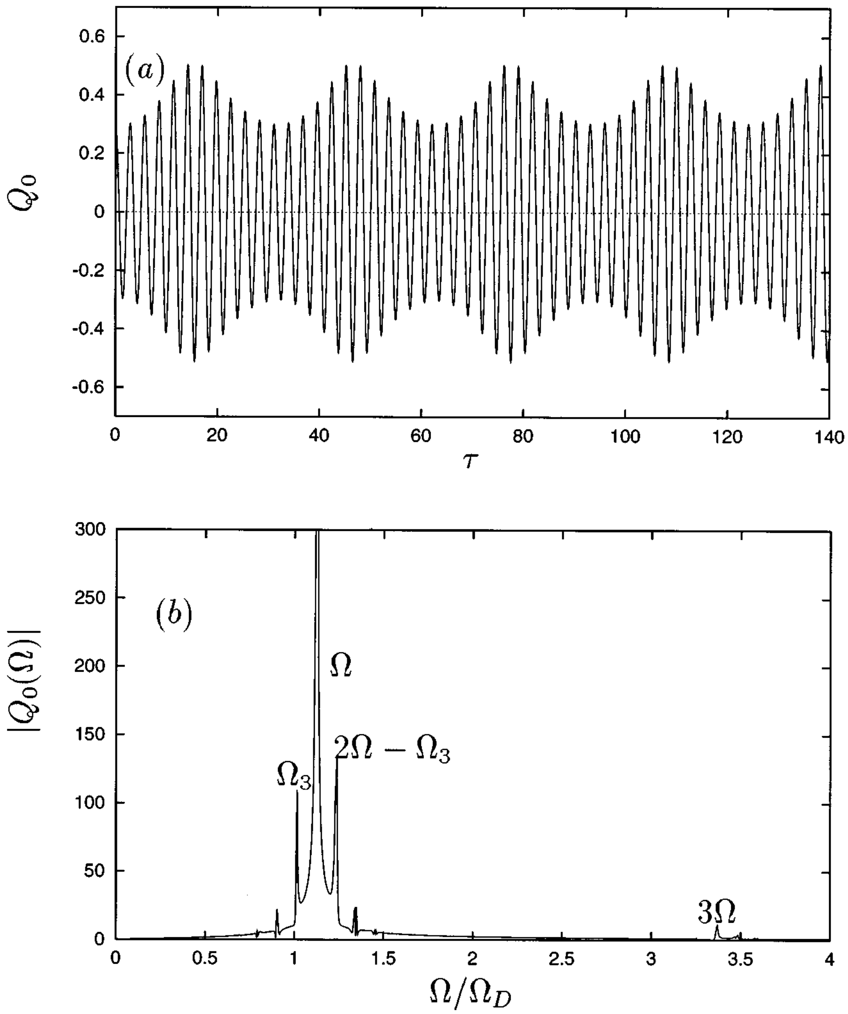

FIG. 2. (a) Displacement Q_0 as a function of time τ obtained for the breathing SLS generated by the initial condition $Q_n(0)=A(-1)^n/\cosh(An)$; $P_n(0)=0$; $A=0.3$. (b) Fourier transform of $Q_0(\tau)$. The peak with frequency Ω has an intensity 3×10^3 (arb. units).

denoted by Ω_3; the notation is explained in Sec. V. The other frequencies which appear in Fig. 2(b) are simple linear combination of Ω and Ω_3 and are discussed in Sec. VI. The amplitude modulation of the central particle and the conservation of the total energy causes a spatial breathing of the SLS. The spatial extension of the SLS changes with time (see Fig. 3) and this breathing behavior is shown in the energy contour plot of Fig. 4.

The main feature of the breathing soliton is the presence of two distinct frequencies in the Fourier transform of the displacement and their generation is also verified with different archetypical excitations, for example with a single-site displacement excitation $[Q_n(0)=A\delta_{n,0};\ P_n(0)=0]$. The spectrum for this case is shown in Fig. 5 which has been found by Zavt.[18] Similarly this is also verified with an external force which acts on a single atom for a limited time.[15,14]

The numerical simulations show that this breathing behavior is a *transient phenomenon*, but it can persist for a very long time (for example, the breathing SLS in the numerical experiment of Fig. 2 survives more than 20 000 fundamental oscillations characterized by the period $T=2\pi/\Omega$). A faster approach to a stationary situation is shown in Fig. 6(a), where we show the maximal value of the displacement at the center of the soliton $Q_0^{\max}$ as a function of the time for an initial condition described by expression (6) with parameter $A=0.2$ and $\mu=0.26$. We observe that the maximal value of the displacement has the tendency to reach a constant value but this process is still requires many time periods. During the evolution the breathing soliton radiates energy in form of small amplitude wave packets [see Fig. 6(b)] and at the end of this stabilization process a SLS with only a single fundamental frequency survives. This phenomenon will be reconsidered in Sec. VI. This type of breathing behavior is found also in other systems, e.g., in Klein-Gordon lattices[19,20] or in sine-Gordon lattices.[21] In the next section we present a study of the two-frequency SLS based on a harmonic model.

V. HARMONIC MODEL FOR THE TWO-FREQUENCY SLS

The nonbreathing SLS in the FPU chain is well described by monochromatic solutions, and their features are essentially the same as those obtained for localized modes in a harmonic chain with force-constant defects. We consider a small deviation from the initial condition $Q_n^0(0)$ which generates a SLS with only a single fundamental frequency Ω. The time evolution than can be described by the ansatz

$$Q_n(\tau)=Q_n^0(\tau)+X_n(\tau), \tag{7}$$

where $Q_n^0(\tau)$ represent the exact solution of the equation of motion (1) for a SLS and $X_n(\tau)$ is a small deviation from the

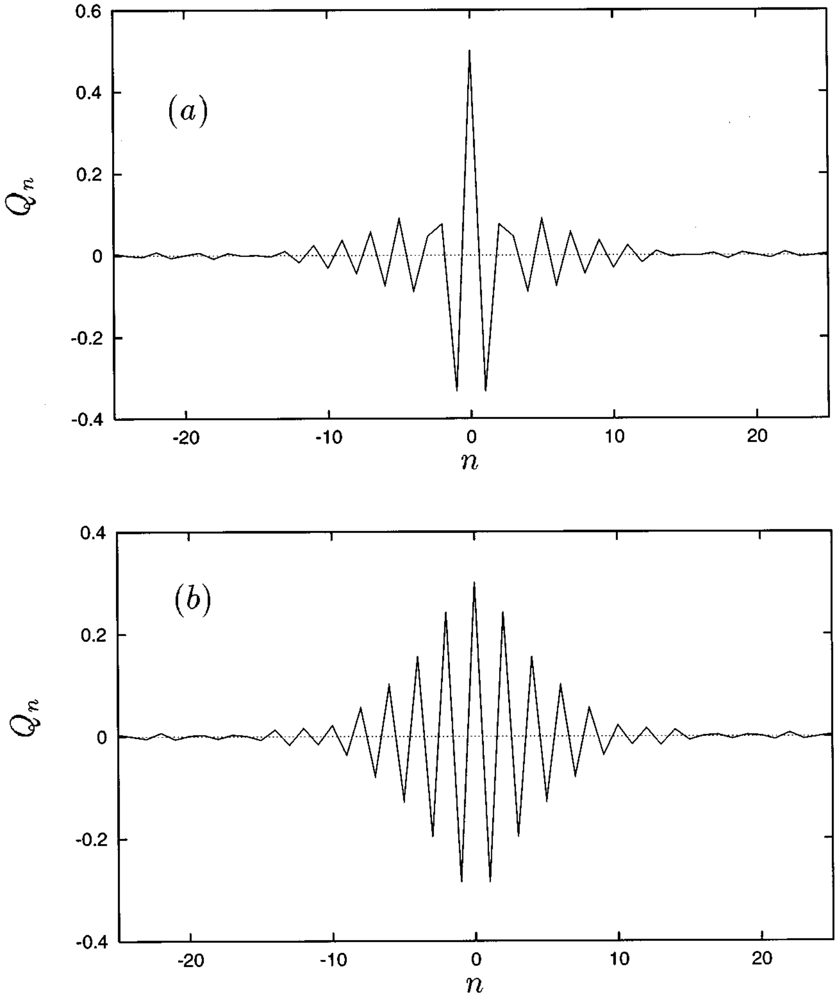

FIG. 3. (a) Displacement pattern Q_n for the breathing soliton of Fig. 2; τ=45. (b) Displacement Q_n for the breathing soliton of Fig. 2; τ=62.

exact solution ($|X_n| \ll |Q_n^0|$). In addition to that we assume that also the following relation is satisfied:

$$|X_n - X_{n+1}| \ll |Q_n^0 - Q_{n+1}^0|. \tag{8}$$

Inserting this ansatz in the equation of motion (1) and linearizing with respect to the small quantity X_n we find the following system of equations:

$$\frac{d^2 X_n}{d\tau^2} = -\sum_{n'=n\pm 1} (X_n - X_{n'})[1 + 3(Q_n^0 - Q_{n'}^0)^2]. \tag{9}$$

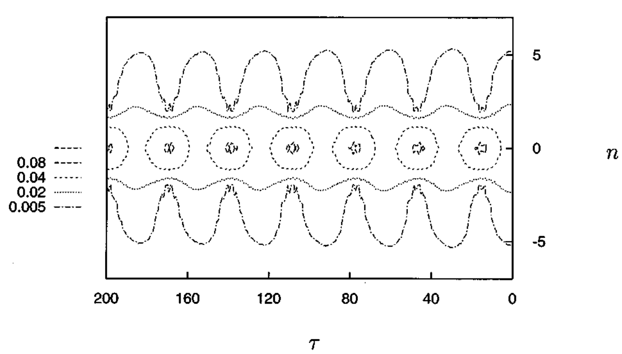

FIG. 4. Energy contour plot for the breathing SLS of Fig. 2.

The exact solution of the equation of motion can be written in the form (all $A_n > 0$):

$$Q_n^0(\tau) = (-1)^n A_n \cos(\Omega\tau) + B_n \cos(3\Omega\tau) + C_n \cos(5\Omega\tau) + \cdots, \tag{10}$$

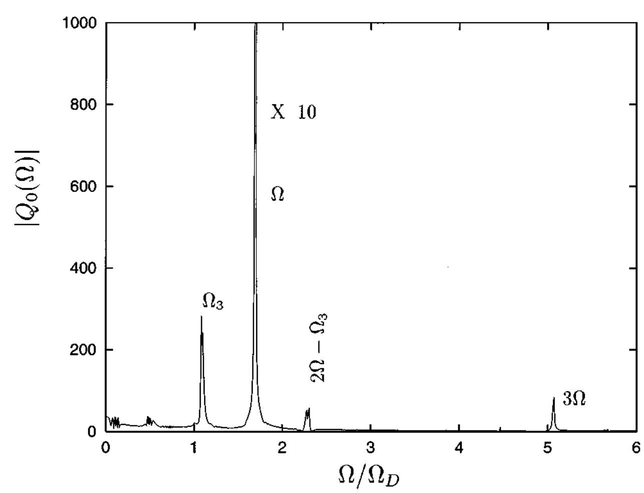

FIG. 5. Fourier transform of $Q_0(\tau)$ for a SLS generated by the initial condition $Q_n(0) = 2\delta_{n,0}$; $P_n(0) = 0$. The peak with frequency Ω has an intensity 10^4 (arb. units).

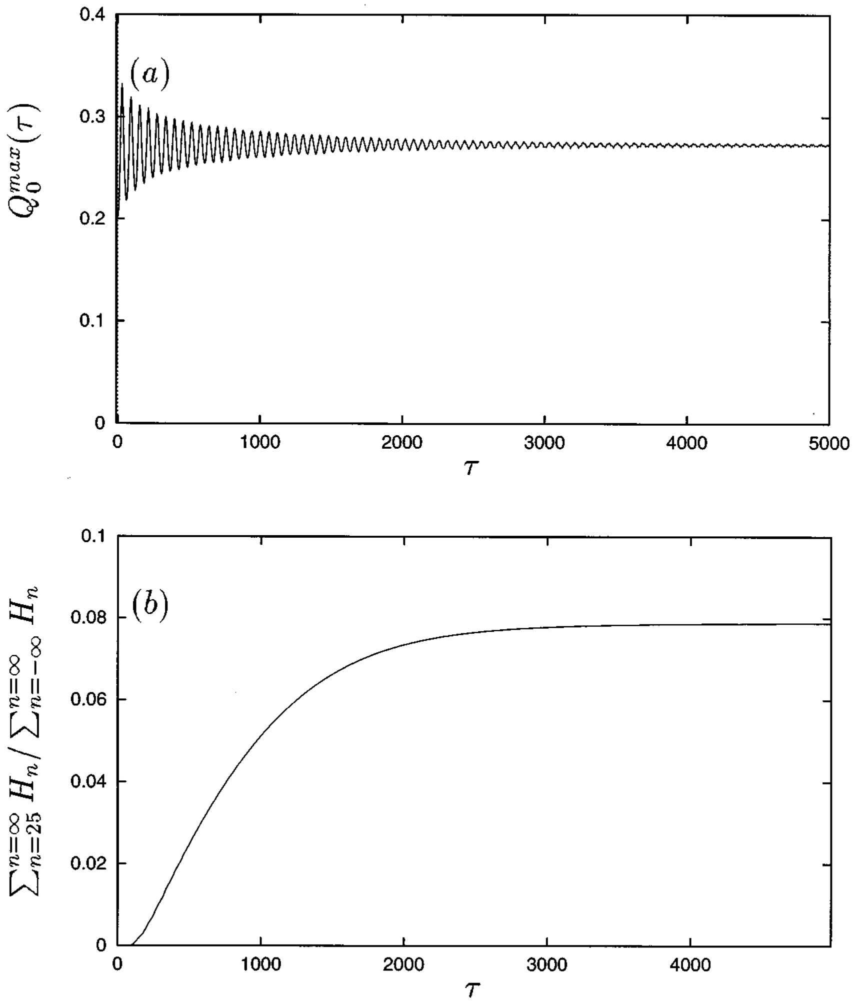

FIG. 6. (a) Maximal value of the amplitude Q_0 as a function of time τ obtained for the initial condition $Q_n(0)=A(-1)^n/\cosh(1.3An)$; $P_n(0)=0$; $A=0.2$; (b) $\Sigma_{n=25}^{\infty}H_n/\Sigma_{n=-\infty}^{\infty}H_n$ as a function of time τ.

where the amplitudes of the different components satisfy the relation $|A_n| \gg |B_n| \gg |C_n| \ldots$ both for small and large anharmonicity.[9,13] This is also shown in Fig. 1 where the component with frequency 3Ω has an intensity of two orders of magnitude smaller than the component with frequency Ω. At this point we discard the high-frequency components on the right-hand side of Eq. (9), i.e., we use in Eq. (9) the approximation $(Q_n^0 - Q_{n'}^0)^2 \simeq (A_n + A_{n'})^2(\cos(\Omega\tau))^2$. This is justified because of the antiphase property of the dominant term in Eq. (10). Substituting then for $Q_n^0(\tau)$ the approximate (monochromatic) solution of the SLS

$$Q_n^0(\tau) = (-1)^n A_n \cos(\Omega\tau), \tag{11}$$

we find the following system of linear equations with periodic coefficients (parametric oscillators):

$$\frac{d^2X_n}{d\tau^2} = -\sum_{n'=n\pm1} (X_n - X_{n'})[1 + 3(A_n + A_{n'})^2(\cos(\Omega\tau))^2]. \tag{12}$$

The functional behavior of this system is characterized by means of the Floquet theory (see, for example, Ref. 22) which is a powerful tool for the stability analysis.[23]

In the present investigation the aim is a first approach to the problem of the breathing SLS in the FPU chain. Therefore, we propose in the following a simplified model, which allows for a qualitative explanation of the phenomenon. The time-dependent ''force constant'' between the sites n and $n+1$ in Eq. (12) is given by

$$f_{n,n+1}(\tau) = 1 + \tfrac{3}{2}(A_n + A_{n+1})^2 + \tfrac{3}{2}(A_n + A_{n+1})^2 \cos(2\Omega\tau). \tag{13}$$

Considering the equation of motion (1) we note that the presence of the nonlinear term, qualitatively causes a hardening of the springs, which is proportional to the squared amplitude of the displacements.

The *main ingredient* of our calculation will be the assumption that it is permissible to investigate localized ''perturbation'' modes provided there are any, and provided their frequency is *considerably lower* than the doubled solitary frequency 2Ω in a harmonic approximation of Eq. (12), replacing the time-dependent ''spring constants'' Eq. (13) by their time-averaged value

$$f_{n,n+1} = 1 + \tfrac{3}{2}(A_n + A_{n+1})^2. \tag{14}$$

If this is done, the equations of motion for the perturbations $X_n(\tau)$ acquire the form of those for a disturbed harmonic lattice with hardened springs in a central region. These equations may have more than a single localized mode with frequency greater than Ω_D. But keeping in mind that in Eq.

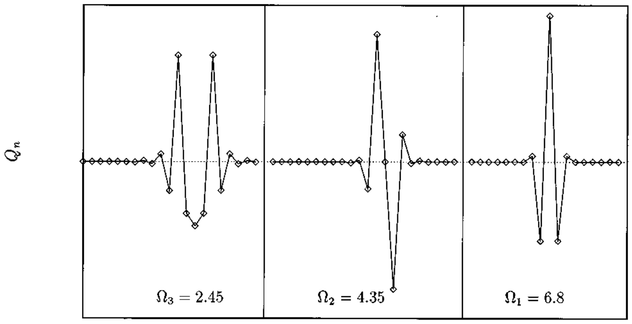

FIG. 7. Eigenvectors with $\Omega>\Omega_D$ for the effective harmonic chain of a SLS ($\gamma_4=4$) with spring distribution Eq. (15).

(13) we have discarded the oscillating term, we stress that only those solutions Ω_i will be of physical relevance, for which $\Omega_i \ll 2\Omega$. E.g., these equations will also produce a frequency Ω_1, which is close to the solitary frequency Ω whence within our concept it must be discarded.

In the present analysis we consider the case of a great anharmonicity ($\gamma_4>1$), since in this case the SLS solution is strongly localized. Consequently, the number of involved degrees of freedom is small and the analysis is more simple. Moreover, in this manner we satisfy the above prerequisite of our model. Referring to approximation (14), we notice that the odd-parity solution described above (see Sec. III) by the displacement pattern $A(0,\ldots,0,-1/2,1,-1/2,0,\ldots 0)$ generates a harmonic spring distribution of the type:

$$f_2(1,\ldots 1,\beta,\alpha,\alpha,\beta,1,\ldots,1), \tag{15}$$

where the spring constants ($\alpha>\beta>1$) are obtained substituting the values of the amplitude of the SLS in Eq. (14). On the other hand, the even-parity solution with displacement pattern $A(0,\ldots 0,-1,1,0,\ldots 0)$ generates a spring distribution

$$f_2(1,\ldots 1,\beta,\alpha,\beta,1,\ldots,1), \tag{16}$$

where $\alpha>\beta>1$.

The eigensolutions of the harmonic chain with spring distribution given by Eq. (15) are shown in Fig. 7 for an odd-parity SLS with $\gamma_4=4$. The eigensolutions are obtained by means of the diagonalization of the dynamical matrix of a harmonic chain with 100 atoms and with spring defects Eq. (15) at the center of the chain. The eigenmodes with frequency greater than Ω_D are extremely localized and their frequencies are practically independent from the length of the chain or from the boundary conditions. There are three localized modes with frequencies above the Debye frequency, two with odd parity (Ω_1 and Ω_3) and one with even parity (Ω_2). The localized mode with frequency Ω_1 has the same form as the odd-parity SLS but this mode has a frequency near to the solitary frequency Ω, and hence according to the above stated presupposition will not be considered.

Thus, we may conclude that, if the solitary solution is disturbed with a small localized perturbation of the same parity, which does not alter the displacement pattern significantly (i.e., the corresponding effective spring distribution), we will find a second peak in the spectrum lying below the SLS frequency, and this second peak can be attributed to the second odd-parity mode Ω_3 found above. On the other hand, if the solitary solution is disturbed with a small perturbation of the opposite parity, we will find another peak which can be attributed to the mode of the effective harmonic chain with frequency Ω_2.

Analogous results are obtained if we consider an even-parity SLS. The SLS can be simulated by a spring distribution given by Eq. (16) and in this case there are two localized modes with even parity denoted by Ω_1 and Ω_3 and another with odd parity and frequency Ω_2. Similarly also here we may consider a weak localized perturbation of opposite parity which generates a peak near Ω_2 or a localized perturbation of the same parity which generates a peak near Ω_3.

VI. DISCUSSION

In this section we first check the validity of our harmonic model by means of numerical simulations. We consider the initial condition given by the displacement pattern Eq. (5) which generates a SLS with only a single fundamental frequency, and we perturb the SLS with a small impulse (P case) or displacement (Q case) perturbation of even or odd parity at the center of the SLS. The results obtained for a small P perturbation are analogous to the results obtained if the perturbation is taken in the Q space. The time evolution of the FPU chain for these ''perturbed'' initial conditions is then calculated by numerical solution of the equation of motion (1).

In Fig. 8(a) we show the displacement $Q_0(\tau)$ at the central site $n=0$ as a function of the time for an odd-parity Q perturbation schematically described by $(\uparrow\cdot\uparrow)$ of the initial condition which would exactly generate the odd-parity SLS of type $(\downarrow\uparrow\downarrow)$ and anharmonicity $\gamma_4=4$. The time evolution shows evidently that the value of the amplitude of the displacement $Q_0(\tau)$ is no longer a constant and new frequencies appear in the Fourier transform [see Fig. 8(b)].

The main effect of the perturbation is the generation of a second frequency corresponding to the odd-parity mode indicated by Ω_3 in Fig. 7. The effective force constants can be calculated if we substitute the values of the amplitudes of the unperturbed SLS in Eq. (14). We obtain a harmonic chain with spring distribution of the type Eq. (15) which has three eigenmodes beyond the Debye frequency and with amplitude pattern shown in Fig. 7. The calculation of the eigenfrequencies give us the value of $\Omega_3=2.45$ which is very close to the frequency $\Omega_3=2.55$ obtained with the numerical simulation [see Fig. 8(b)].

The other frequencies which appear in the Fourier transform are linear combination of the frequencies Ω and Ω_3 and are due to a nonlinear coupling of the two modes. If we consider a trial solution of the form

$$Q_n = A_n e^{i\Omega\tau} + B_n e^{i\Omega_3\tau} + \text{c.c.}, \tag{17}$$

where A_n and B_n are the amplitude distributions, respectively, of the SLS with frequency Ω and of the localized mode with frequency Ω_3, the substitution of this trial solution in the equation of motion (1) shows that also terms with frequencies $2\Omega\pm\Omega_3, 2\Omega_3\pm\Omega\ldots$ must appear in the solution. This indeed is observed in the numerical simulation [see Fig. 8(b)].

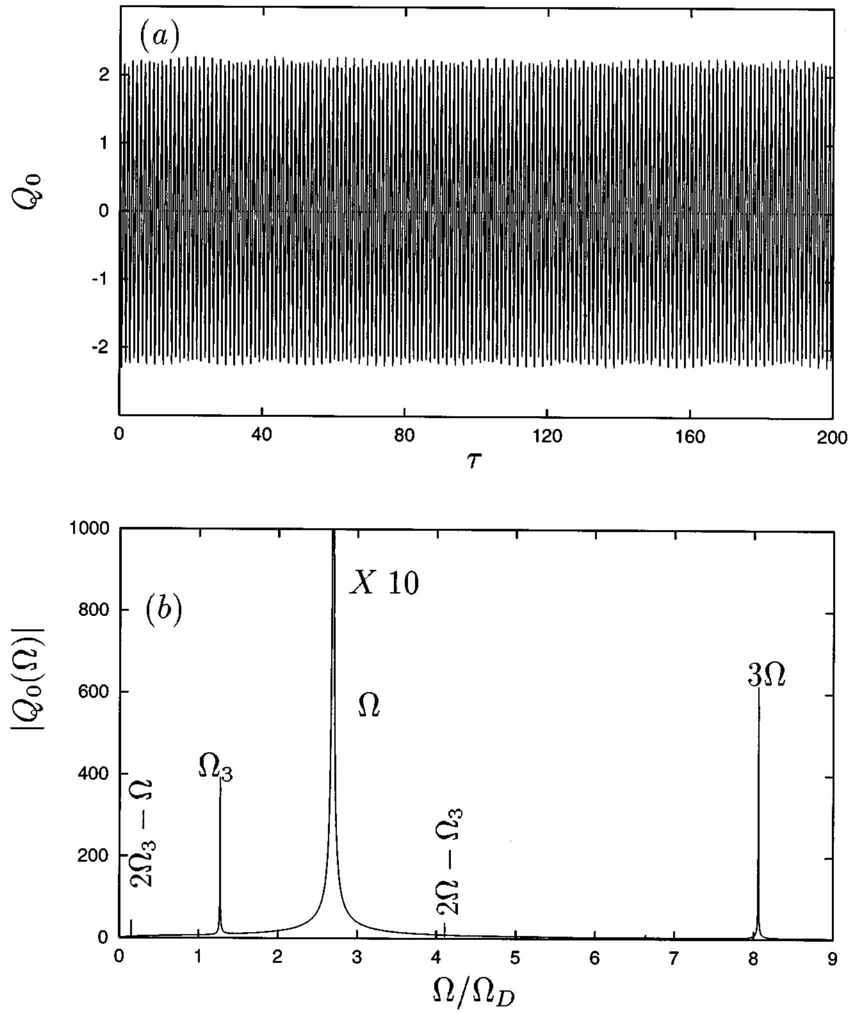

FIG. 8. (a) Displacement Q_0 as a function of time τ obtained for the breathing SLS generated by an odd-parity perturbation of the odd-parity mode with $\gamma_4=4$. Initial condition: $Q_n(0)=2$ $(...,0,0.055,-0.54,1,-0.54,0.055,0,...)+0.3$ $(...,0,-1,0,-1,0,...)$; $P_n(0)=0$. (b) Fourier transform of $Q_0(\tau)$. The peak with frequency Ω has an intensity 10^4 (arb. units).

At this point we now return to the breathing SLS mentioned in Sec. IV (see Fig. 6) and its decay. At present there is no numerical evidence of the existence of a stable two-frequency SLS in the FPU chain, but the numerical simulations have confirmed the persistence of the two-frequency solution for a very long lifetime. As suggested by Boesch and Peyrard for the sine-Gordon chain,[21] the decay of the breathing SLS can be explained by means of an external parametrical resonance with phonons. This can be visualized in the following manner. The breathing SLS is described by two different frequencies above the Debye frequency, but the nonlinear term in the equation of motion causes the appearance of linear combinations of these two frequencies in the spectrum. Then, if one of these linear combinations lies in the phonon band, we expect an energy radiation caused by the parametric resonance (Fano decay).[24] This indeed is confirmed in our numerical experiments where the generation of small amplitude phonon packets is observed.

Whereas the odd-parity SLS is stable to odd-parity perturbations, as shown by Sandusky *et al.*[12] and independently by Chubykalo *et al.*[13] via a stability analysis, this is not true for an even-parity perturbation described schematically by $(\uparrow.\downarrow)$. The even-parity perturbations destroy the symmetry and cause the SLS to move. Its mean position may travel in space or oscillate around a central position.[12] Consequently, there is a great fluctuation in the displacement pattern, and the effective harmonic spring distribution is no longer described by Eq. (15). Our harmonic model cannot describe this phenomenon, since the effective spring distribution is assumed to be static.

The even-parity SLS is stable against both small even-parity and odd-parity perturbations,[12,13] and for this type of SLS our harmonic model gives a good explanation of the breathing behavior induced by a perturbation. The properties of the even-parity SLS is also discussed in the paper of Flach and Willis,[10] where the existence of a movability separatrix is demonstrated. If the odd-parity perturbation is greater than a threshold value, the SLS transforms into a moving SLS. For our numerical simulations the odd-parity perturbation is always chosen sufficiently small, such that the SLS remains localized at the same position, maintaining approximately the original displacement pattern. Only for such a choice our harmonic model for the breathing SLS is applicable.

In Fig. 9(a) we show the time evolution of the energy center defined by $\Sigma_n nH_n/\Sigma_n H_n$ as a function of time for an even-parity SLS with $\gamma_4=4$ [schematically described by $(\uparrow\downarrow)$] which is perturbed by a small odd-parity impulse perturbation $(\uparrow\uparrow)$. In this case the perturbation destroys the symmetry of the SLS, and the energy center oscillates around its mean value of 0.5. We observe the appearance of a new frequency Ω_2 in the spectrum of the displacement [see Fig. 9(b)] caused by the perturbation. This fact can be explained

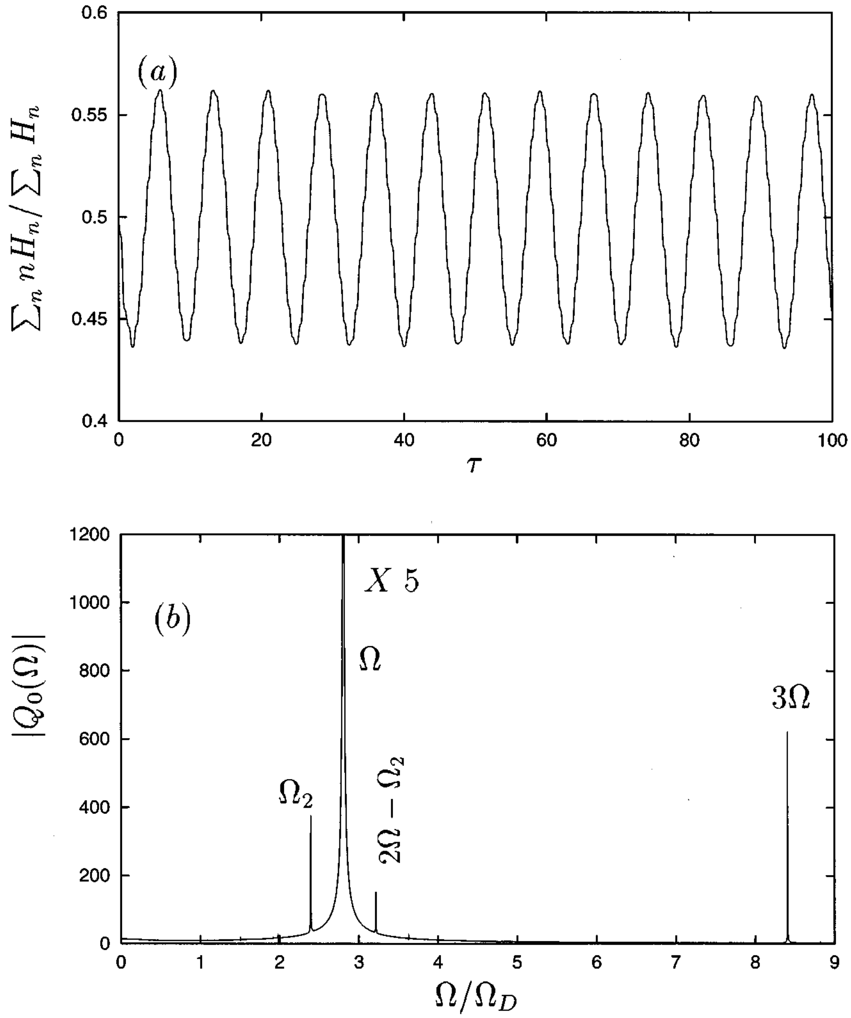

FIG. 9. (a) Energy center $\Sigma_n nH_n/\Sigma_n H_n$ as a function of time τ obtained for the breathing SLS generated by the appropriate initial condition for the even-parity mode with $\gamma_4=4$ which is perturbed by an odd-parity perturbation in *P space*. Initial conditions: $Q_n(0)=2(...,0,0.21,-1,1,-0.21,0,...)$; $P_n(0)=0.3(...,0,0,1,1,0,0,...)$. (b) Fourier transform of $Q_0(\tau)$. The peak with frequency Ω has an intensity 6×10^3 (arb. units).

if we assume that the odd-parity perturbation activates the odd-parity mode with frequency Ω_2 which appears in our harmonic model. Also the spatial oscillation of the energy center finds a simple explanation within our harmonic model. Indeed, a superposition of the odd-parity mode with frequency Ω_2 and of the even-parity SLS [see Eq. (7)] causes an oscillation of the energy center around its mean value.

On the other hand, if we consider an even-parity perturbation of the even parity SLS, described schematically by $(\downarrow..\uparrow)$, the main effect of the perturbation is the activation of the even-parity mode indicated by Ω_3. The results of the numerical simulation are shown in Fig. 10. In this case we have again a breathing type of behavior. For the even parity SLS, the eigenfrequencies of the corresponding harmonic chain ($\Omega_2=4.5$, $\Omega_3=3.0$) are very close to the frequencies obtained by the numerical simulations ($\Omega_2=4.8$, $\Omega_3=3.1$). The same analysis performed for other values of the anharmonicity parameter confirms the validity of our harmonic model. For example, for the even parity SLS with $\gamma_4=9$ the eigenfrequencies calculated with our model are $\Omega_2=6.4$, $\Omega_3=4.2$ and the frequencies obtained by numerical simulations are $\Omega_2=6.8$, $\Omega_3=4.2$.

It should be noted that the frequencies obtained by a small localized perturbation depend only on the parity of the perturbation and are independent from the chosen displacement pattern (or impulse pattern) of the particular perturbation. For example, in the case of an even-parity SLS, a small odd-parity perturbations described by $(.\uparrow\uparrow.)$ generates the same frequency as a perturbation of type $(\uparrow..\uparrow)$ or of type $(\downarrow\uparrow\uparrow\downarrow)$. This fact indicates that the nonbreathing SLS establishes well determined internal degrees of freedom, and their excitation depend only on the parity of the perturbation. This is well reproduced by our harmonic model.

VII. CONCLUSION

In this paper we present a study of the breathing self-localized soliton in the FPU chain. The main characteristics of the breathing SLS is the presence of two distinct frequencies in the Fourier transform of the displacements and a spatial envelope which displays a breathing behavior. The generation of the breathing SLS is investigated by means of numerical experiments. We have shown that the breathing SLS can be generated with different types of archetypical excitations, for example with a single site displacement excitation or with an external force which acts on a single site for a limited time.[14,15] These breathing solitons are not stable in time, but the numerical simulations have shown a breathing behavior which can persist for a very long time.

To understand this type of behavior we have proposed a harmonic model for the breathing SLS. The original nonbreathing SLS is well described by a monochromatic solu-

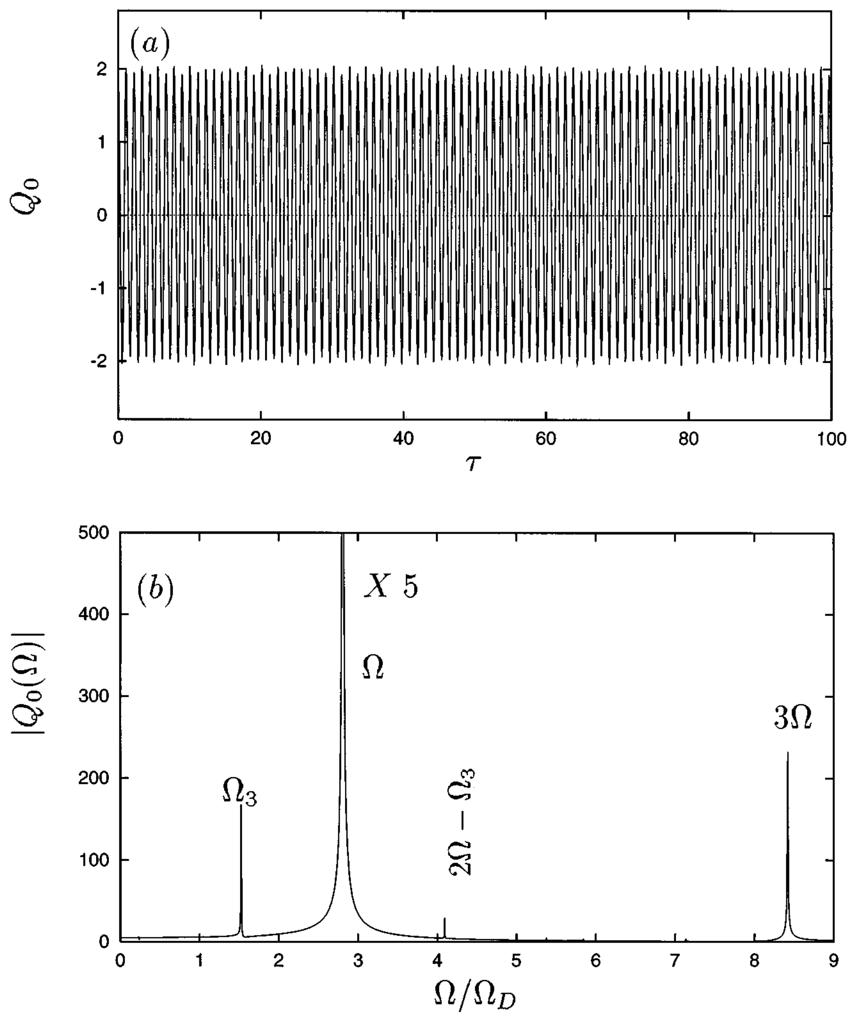

FIG. 10. (a) Displacement Q_0 as a function of time τ obtained for the breathing SLS generated by the appropriate initial condition for the even-parity mode with $\gamma_4=4$ which is perturbed by an even-parity perturbation in *P space*. Initial conditions: $Q_n(0)=2(\ldots,0,0.21,-1,1,-0.21,0,\ldots)$; $P_n(0)=0.8(\ldots,0,-1,0,0,1,0,\ldots)$. (b) Fourier transform of $Q_0(\tau)$. The peak with frequency Ω has an intensity 2.5×10^3 (arb. units).

tion with a constant displacement pattern. In this model the presence of the nonlinear term in the equation of motion causes an effective hardening of the springs, which is proportional to the squared amplitude of the displacements. The dominant philosophy of our model rests on the concept that the SLS establishes an effective spring distribution for additional small-amplitude localized motions of harmonic nature.

In our investigation we have considered the case of great anharmonicity, where the SLS's are strongly localized. For the even- and odd-parity SLS's we have shown that the corresponding effective harmonic chain gives rise to different localized modes with frequencies above the Debye frequency and with different parity. The respective localized mode with highest frequency Ω_1 reproduces the displacement pattern of the SLS but it does not reproduce the correct frequency value Ω of the SLS, since its calculation violates the presupposition ($\Omega_i \ll 2\Omega$) of our model. But there are two other modes, one with opposite parity and another one with the same parity as the SLS, which both have frequencies greater than the Debye frequency and which satisfy the presupposition $\Omega_i \ll 2\Omega$. These modes can be viewed as internal degrees of freedom of the SLS and can be excited if we perturb the original SLS with, respectively, a small odd-parity perturbation or an even-parity perturbation.

To check the validity of our model we have employed numerical experiments. It has turned that the numerical values of the new frequencies are very close to those found in our analytical model. They differ in the chosen examples by less than 7% and are improved for ascending values of anharmonicity γ_4.

The results of our numerical simulations show that the perturbed SLS has a breathing behavior and there is the appearance of a new frequency in the Fourier transform of the displacement. Our harmonic model can explain the breathing behavior as a superposition of the unperturbed SLS and of a localized mode of the corresponding effective harmonic chain. The slow decay of the breathing SLS is explained by means of an external parametrical resonance with phonons.

A more accurate analysis of the considered breathing phenomenon can be obtained considering the system of linear equations with periodic coefficients given by Eq. (12). This will be considered in the near future.

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[1] A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, *Theory of Lattice Dynamics in the Harmonic Approximation*, 2nd ed. (Academic, New York, 1971).
[2] A. S. Dolgov, Sov. Phys. Solid State **28**, 907 (1986).
[3] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[4] R. Bourbonnais and R. Maynard, Phys. Rev. Lett. **64**, 1397 (1990).
[5] V. M. Burlakov, S. A. Kiselev, and V. N. Pyrkov, Solid State Commun. **74**, 327 (1990).
[6] S. Takeno, K. Kisoda, and A. J. Sievers, Prog. Theor. Phys. Suppl. **94**, 242 (1988).
[7] J. B. Page, Phys. Rev. B **41**, 7835 (1990).
[8] K. Yoshimura and S. Watanabe, J. Phys. Soc. Jpn. **60**, 82 (1991).
[9] S. R. Bickham and A. J. Sievers, Phys. Rev. B **43**, 2339 (1991).
[10] S. Flach and C. R. Willis, Phys. Rev. Lett. **72**, 1777 (1994).
[11] R. Dusi and M. Wagner, Phys. Rev. B **51**, 15 847 (1995).
[12] K. W. Sandusky, J. B. Page, and K. E. Schmidt, Phys. Rev. B **46**, 6161 (1992).
[13] O. A. Chubykalo, A. S. Kovalev, and O. V. Usatenko, Phys. Lett. A **178**, 129 (1993).
[14] R. Dusi, G. Viliani, and M. Wagner, Philos. Mag. B **71**, 597 (1995).
[15] R. Dusi, *Tesi di laurea in fisica* (Universita' degli studi di Trento, 1993).
[16] E. Fermi, *Collected Papers*, Vol. 2 (University of Chicago Press, Chicago, 1965).
[17] J. Ford, Phys. Rep. **213**, 271 (1992).
[18] G. S. Zavt (private communication).
[19] S. Flach, C. R. Willis, and E. Olbrich, Phys. Rev. E **49**, 836 (1994).
[20] T. Dauxois, M. Peyrard, and C. R. Willis, Phys. Rev. E **48**, 4768 (1993).
[21] R. Boesch and M. Peyrard, Phys. Rev. B **43**, 8491 (1990).
[22] A. H. Nayfeh and D. T. Mook, *Nonlinear Oscillations* (Wiley, New York, 1979).
[23] K. W. Sandusky and J. B. Page, Phys. Rev. B **50**, 866 (1994).
[24] M. Wagner and J. Vazquez-Marquez, J. Phys. A **21**, 4347 (1988).