Localized modes in inhomogeneous one-dimensional anharmonic lattices

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We present numerical calculations for the determination of localized modes in one-dimensional finite chains of atoms with free ends containing harmonic and quartic anharmonic interactions. By adding step by step the quartic term we can follow the formation of even and odd localized modes arising from the highest harmonic frequency mode. We have studied the role of crystal inhomogeneity by introducing a modification of the fourth-order force constant between neighboring atoms at the center of the chain, where the localized mode has its maximum displacement. For large weakening of this force constant the localized mode develops a double-peaked structure, as has been found in the continuum limit. In the case of asymmetrical local inhomogeneity the localized mode remains stable and moves toward the atom with the inhomogeneity. We also show the existence of anharmonic surface modes localized at the end of the chain.

I. INTRODUCTION

In recent years interest in the study of the anharmonicity of crystals has increased considerably. Some examples of properties of solids which are mainly or partly determined by crystal anharmonicity are specific heat at high temperatures, melting, thermal expansion, temperature dependence of the elastic constants, and damping of high-frequency sound waves. Anharmonicity is also of importance in defect properties of crystals because displacements are often large near imperfections.

Recent theoretical studies of the lattice dynamics of strongly anharmonic crystals[1-8] have shown the existence of localized modes with frequencies above the maximum frequency of the harmonic crystal. These modes resemble those associated with point defects or vacancies in harmonic crystals.[9,10] Sievers and Takeno[2] obtained analytically this new kind of localized mode, in homogeneous anharmonic crystals, by studying classical systems in the rotating-wave approximation[11] (RWA), i.e., by including in the time dependence of the displacements a single-frequency component. These modes, which exist in perfect lattices and are strongly localized on a lattice site, can appear at any lattice site because of translational invariance. It was argued that this incoherent disorder produces a configurational entropy term that has to be considered in a complete thermodynamic description of the anharmonic crystal properties. These modes were called intrinsic localized modes by Sievers and Takeno[2] in order to distinguish them from the impurity induced localized modes. The Sievers-Takeno modes have odd parity. Similar modes of even parity have been reported by Page.[4] It is of interest to see how these intrinsic localized modes are modified in an inhomogeneous system. This problem has been studied analytically by Kivshar[12] by considering a mass defect. He showed that the impurity modes can be treated as intrinsic localized modes on the impurity site. Also, a nonlinear thin film covering a surface can give rise to localized modes.[13,14]

In this paper we examine the effects on the intrinsic localized modes produced by a local modification of the anharmonic part of the force field between atoms. Our aim is to show the existence of localized modes for this kind of inhomogeneous system. We treat the problem numerically by solving the equations of motion of a linear monatomic chain of a sufficiently large number of atoms N in such a way that the results do not depend significantly on N.

In Sec. II, we show that by switching on the anharmonic term the upper harmonic mode becomes localized on a few lattice sites and it becomes narrower as we increase the strength of the anharmonic term. In Sec. III, we consider how the intrinsic mode is modified by weakening or by increasing the anharmonic force constant acting on the lattice sites corresponding to the maximum displacement. We consider the case of even- and odd-parity modes and we show that for a strong weakening of the fourth-order anharmonic interactions the displacement maximum of an intrinsic localized mode splits into two peaks, one on the left and the other on the right of the lattice site of maximum displacement of the initial intrinsic mode. This situation is similar to that described by Kivshar[12] in the continuum limit, where a suitable change of the impurity mass gives rise to a splitting of the displacement maximum of a soliton mode into two peaks localized symmetrically about the impurity. In Sec. IV, we consider the case of moving the modified anharmonic force constant away from the maximum of the intrinsic mode. In this case we notice a tendency of the odd localized mode to move away from the initial position toward the atom with modified force constant. Section V is devoted to the study of surface modes. We show the existence of localized modes close to the end of the chain.

In the case of pure quartic interactions two modes exist, one of the type $(-0.165,1,-1,0.166,\ldots)$ which looks like an even mode and the other similar to an odd mode. The inclusion of a weak harmonic interaction produces a slight distortion of the pattern of the modes. The final conclusions are drawn in Sec. VI.

II. THEORETICAL MODEL

The study of nonlinear systems often reduces to the analysis of one-dimensional models, as for instance solitons in optical fibers, effects of lattice-dynamical anharmonicity on multilayered structures, dislocations in crystals, etc. For this reason and to greatly simplify the problem we consider a one-dimensional monatomic chain of particles interacting via nearest neighbors with harmonic and quartic anharmonic interactions. The Hamiltonian has the form

$$H=\tfrac{1}{2}m\sum_n \dot{u}_n^2+\tfrac{1}{2}K_2\sum_n (u_n-u_{n+1})^2 +\tfrac{1}{4}K_4\sum_n (u_n-u_{n+1})^4 , \tag{1}$$

where m is the mass of the particles and u_n is the longitudinal displacement of the nth atom. The equations of motion are easily found to be

$$m\ddot{u}_n+K_2(2u_n-u_{n+1}-u_{n-1}) +K_4[(u_n-u_{n+1})^3+(u_n-u_{n-1})^3]=0 . \tag{2}$$

We seek stationary solutions of the type

$$u_n=A\xi_n\cos(\omega t) . \tag{3}$$

The ξ_n are the relative displacements of the atoms and A is the overall amplitude that can be fixed by the initial boundary conditions. Substituting Eq. (3) into Eq. (2) we obtain

$$m\omega^2 A\xi_n\cos(\omega t)=K_2 A[2\xi_n-\xi_{n+1}-\xi_{n-1}]\cos(\omega t) +K_4 A^3[(\xi_n-\xi_{n+1})^3 +(\xi_n-\xi_{n-1})^3]\cos^3(\omega t) . \tag{4}$$

This equation can also be derived by considering the factored form of the displacements of Eq. (3) and by setting to zero the total time derivative of the total energy of Eq. (1). This alternative procedure gives

$$\tfrac{1}{2}mA^2\omega^2\left[\sum_n \xi_n^2\right]2\omega\sin(\omega t)\cos(\omega t)-\tfrac{1}{2}K_2A^2\left[\sum_n(\xi_n-\xi_{n+1})^2\right]2\omega\sin(\omega t)\cos(\omega t) -\tfrac{1}{4}K_4A^4\left[\sum_n(\xi_n-\xi_{n+1})^4\right]4\omega\sin(\omega t)\cos^3(\omega t)=0 . \tag{5}$$

Since Eq. (5) should coincide with Eq. (4) we get the identities[8]

$$\frac{\sum_n(\xi_n-\xi_{n+1})^2}{\sum_n\xi_n^2}=\frac{2\xi_n-\xi_{n+1}-\xi_{n-1}}{\xi_n} , \tag{6a}$$

$$\frac{\sum_n(\xi_n-\xi_{n+1})^4}{\sum_n\xi_n^2}=\frac{(\xi_n-\xi_{n+1})^3+(\xi_n-\xi_{n-1})^3}{\xi_n} . \tag{6b}$$

To make the equations of motion, Eq. (4), linear in $\cos(\omega t)$, we use the rotating-wave approximation, i.e., we linearize the $\cos^3(\omega t)$ factor as follows:

$$\cos^3(\omega t)\simeq\tfrac{3}{4}\cos(\omega t) . \tag{7}$$

In this way we are left with the equations of motion

$$m\omega^2\xi_n=K_2[2\xi_n-\xi_{n+1}-\xi_{n-1}] +\frac{3K_4A^2}{4}[(\xi_n-\xi_{n+1})^3+(\xi_n-\xi_{n-1})^3] . \tag{8}$$

Having performed the RWA we can integrate back the equations of motion of Eq. (5) to obtain an approximate expression for the total energy:

$$E=\tfrac{1}{2}mA^2\omega^2\left[\sum_n\xi_n^2\right]\sin^2(\omega t) +\tfrac{1}{2}K_2A^2\left[\sum_n(\xi_n-\xi_{n+1})^2\right]\cos^2(\omega t) +\frac{1}{2}\frac{3K_4A^4}{4}\left[\sum_n(\xi_n-\xi_{n+1})^4\right]\cos^2(\omega t) . \tag{9}$$

This equation represents the energy of a fictitious oscillator which oscillates periodically in time. Because of the conservation of energy we have

$$E=\tfrac{1}{2}mA^2\omega^2\sum_n\xi_n^2 \quad \text{for } t=\frac{\pi}{2\omega} , \tag{10a}$$

$$E=\tfrac{1}{2}K_2A^2\sum_n(\xi_n-\xi_{n+1})^2 +\frac{1}{2}\frac{3K_4A^4}{4}\sum_n(\xi_n-\xi_{n+1})^4 \quad \text{for } t=0 . \tag{10b}$$

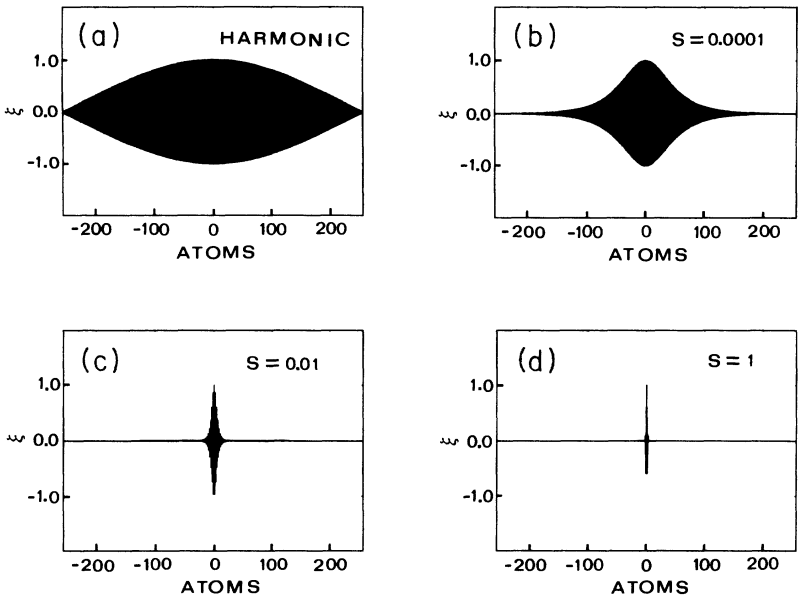

FIG. 1. Odd-parity localized modes. (a) shows the displacement pattern of the highest harmonic mode of a free-end one-dimensional chain of 513 atoms. For clarity the longitudinal displacements have been drawn vertically. (b) shows the odd localized mode of a chain with small anharmonicity ($S=0.0001$), (c) refers to the case $S=0.01$, and (d) to the case $S=1$.

This expression for the total energy will be used in the next section when we introduce a local modification of the fourth-order anharmonic force constants. Here we notice that it depends explicitly on the amplitude A.

We now show numerically that the intrinsic localized modes arise from the highest-frequency harmonic mode when the anharmonicity is switched on. The anharmonicity is measured by the parameter $S=(3/4)(K_4/K_2)A^2$. We start by considering odd-parity solutions for which $\xi_n=\xi_{-n}$. The normalization of the relative displacements pattern is given by choosing $\xi_0=1$. We take a linear chain of 513 atoms, so that $n=-256,\ldots,-1,0,1,\ldots,256$, with free-end boundary conditions. The pattern of the harmonic displacements is presented in Fig. 1(a). For clarity we draw the longitudinal displacements vertically. To solve the system of nonlinear equations in Eq. (8) we use a standard routine based on the Newton scaled gradient. Given an initial guess of the displacements, through an iterative procedure the routine determines the stable solution for each value of the parameter S. We found that convergence in the iterative procedure can be obtained by starting from the purely harmonic solution, whose pattern of harmonic displacements is presented in Fig. 1(a), and then introducing the anharmonicity in small steps. For example, the value of $S=10^{-4}$ presented in Fig. 1(b) is

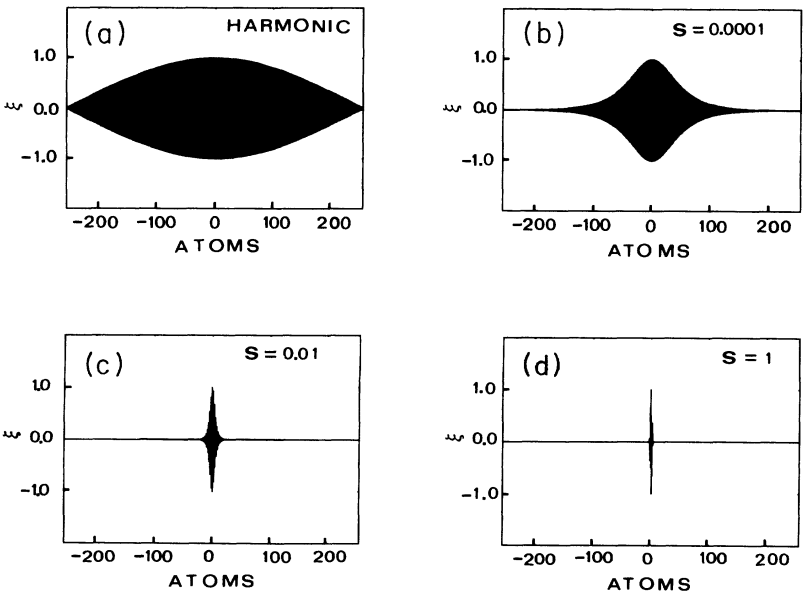

FIG. 2. Even-parity localized modes. (a) shows the displacement pattern of the highest harmonic mode of a free-end one-dimensional chain of 512 atoms. (b) shows the even localized mode of a chain with small anharmonicity ($S=0.0001$), (c) refers to the case $S=0.01$, and (d) to the case $S=1$.

reached in 100 steps. At each step we start with the stable displacement pattern obtained at the previous one, and when the convergence is reached, we pass to the next step. In Fig. 1(b), it is clearly seen that even for a small value of the anharmonicity the mode starts to become localized. By increasing the anharmonicity as shown in Fig. 1(c), corresponding to $S=10^{-2}$, the mode tends to become narrower and for $S=1$ [Fig. 1(d)] it is localized on very few atoms at the center of the chain. For a purely anharmonic chain ($S\rightarrow\infty$) we get a displacement pattern $(\ldots,0.023,-0.523,1,-0.523,0.023,\ldots)$ which is very close to the analytic result $(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$ obtained for anharmonicity order $r\rightarrow\infty$. We have also studied the even-parity localized modes ($\xi_n=-\xi_n$). In this case it is convenient to change the particle labeling in such a way that there is no particle at $n=0$. The normalization requirement is $\xi_{-1}=1$ and the parity of the solution gives as a consequence $\xi_1=-1$. We performed calculations for a chain of 512 atoms, starting from the same harmonic solution as for the odd modes [Fig. 2(a)], increasing the anharmonicity parameter S in the same sequence. In Fig. 2(b) is drawn the resulting pattern for $S=10^{-4}$, in Fig. 2(c) the pattern for $S=10^{-2}$ and in Fig. 2(d) the $S=1$ case. As one can see, the even modes also become more and more localized with increasing anharmonicity parameter S. In the fully anharmonic case we get the displacement pattern $(\ldots,0,+0.166,-1,+1,-0.166,0,\ldots)$ which is very close to the analytic solution $(\ldots,0,+\frac{1}{6},-1,1,-\frac{1}{6},0,\ldots)$ obtained for anharmonicity order $r\rightarrow\infty$.

III. INHOMOGENEOUS LINEAR CHAIN: SYMMETRIC LOCAL INHOMOGENEITY

We now consider a local modification of the fourth order force constant K_4. We start by considering the even-parity modes. We first consider a modification of the force constant K_4 between the atomic sites with the maximum displacement (sites $n=-1$ and $n=+1$), as illustrated in Fig. 3. The equations of motion for this inhomogeneous linear chain with free ends are

$$
\begin{aligned}
&\Omega^2\xi_{-256}=(\xi_{-256}-\xi_{-255})+S[(\xi_{-256}-\xi_{-255})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-n}=(2\xi_{-n}-\xi_{-n+1}-\xi_{-n-1})+S[(\xi_{-n}-\xi_{-n+1})^3+(\xi_{-n}-\xi_{-n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-2}=(2\xi_{-2}-\xi_{-1}-\xi_{-3})+S[(\xi_{-2}-\xi_{-1})^3+(\xi_{-2}-\xi_{-3})^3]\\
&\Omega^2\xi_{-1}=(2\xi_{-1}-\xi_{-2}-\xi_{+1})+S(\xi_{-1}-\xi_{-2})^3+S'(\xi_{-1}-\xi_{+1})^3\\
&\Omega^2\xi_{+1}=(2\xi_{+1}-\xi_{-1}-\xi_{+2})+S(\xi_{+1}-\xi_{+2})^3+S'(\xi_{+1}-\xi_{-1})^3\\
&\qquad\vdots\\
&\Omega^2\xi_{+n}=(2\xi_{+n}-\xi_{+n+1}-\xi_{+n-1})+S[(\xi_{+n}-\xi_{+n+1})^3+(\xi_{+n}-\xi_{+n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{+256}=(\xi_{+256}-\xi_{+255})+S[(\xi_{+256}-\xi_{+255})^3]\ ,
\end{aligned}
\tag{11}
$$

where $\Omega^2=m\omega^2/K_2$. The normalization condition chosen requires $\xi_{-1}=1$. The parameter $S'=(3/4)(K_4'/K_2)A^2$ characterizes the inhomogeneity of the lattice. As in the previous section, to obtain results that are essentially independent of the number N of atoms in the chain, we use 512 atoms. For a fixed value of S, decreasing S', we determine for each value of S' the displacement pattern $\{\xi_n\}$, by starting from the anharmonic solution corresponding to $S=S'$ previously de-

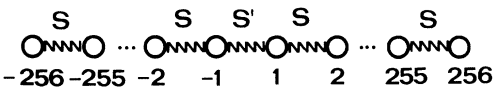

FIG. 3. Sketch of the anharmonic interactions in the free-end inhomogeneous one-dimensional chain of 512 atoms. S refers to unmodified force constants and S' to the modified force constant between the atoms -1 and $+1$ at the center of the chain.

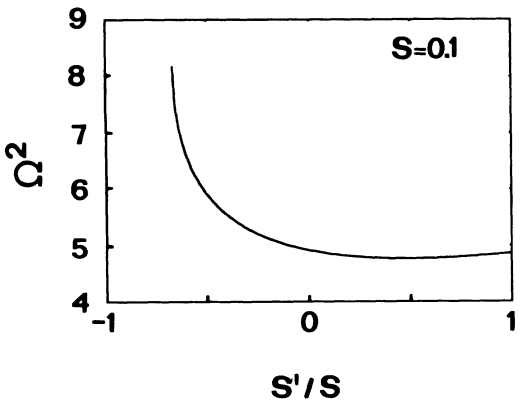

FIG. 4. Frequency squared of even-parity modes for $S=0.1$ as a function of the force constant ratio S'/S.

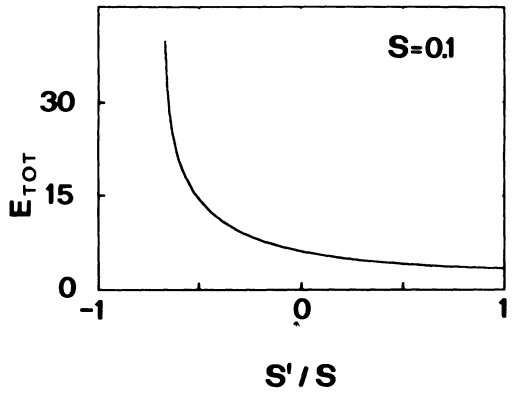

FIG. 5. Total energy of even-parity modes evaluated with Eq. (10a) for $S=0.1$ as a function of the force-constant ratio S'/S.

rived from the highest harmonic mode. Figure 4 shows the results for the frequencies of the stationary even modes as a function of S'/S for the value of $S=0.1$. By decreasing S', Ω^2 starts to decrease, reaches a minimum, and then increases. This behavior is clearly understood by noting that $\Omega^2 \propto S(\xi_{-1}-\xi_{-2})^3+S'(\xi_{-1}-\xi_1)^3$. A decrease of S' produces an increase of the displacement at $n=-2$. In the interval $0.5<S'/S<1$ the decrease of S' dominates because the moduli of ξ_1 and ξ_{-1} are both equal to one, so that Ω^2 decreases, while for smaller values of S'/S the modulus of the displacement at $n=-2$ becomes greater than one and Ω^2 increases. The behavior of the total energy of Eq. (10a) as a function of S'/S is presented in Fig. 5. Note that the spreading of the localized mode that occurs with decreasing S'/S balances the decreasing of Ω^2 through the factor $\sum_n \xi_n^2$, so that the minimum in E is much less pronounced than in the Ω^2 versus S'/S diagram. At a certain point as S'/S decreases, the original intrinsic mode tends to develop a double-peaked structure with maximum displacement at $n=\pm 2$, as shown in Fig. 6. Our iterative procedure can be carried out also for small negative values of S'/S (anharmonic repulsive forces). In Fig. 6(d) is shown the case $S'/S=-0.67$ that clearly shows double-peaked structure, which corresponds to a rise of Ω^2 to nearly vertical in Fig. 4. This phenomenon is very similar to the splitting of the soliton mode peak produced by a mass defect impurity found by Kivshar.[12] We present in Fig. 7 the behavior of Ω^2 as a function of S'/S for a large value of the anharmonicity ($S=10$). Note that in this case the slope of the curve tends to approach infinity at $S'/S=0.0474$, where the intrinsic localized mode devel-

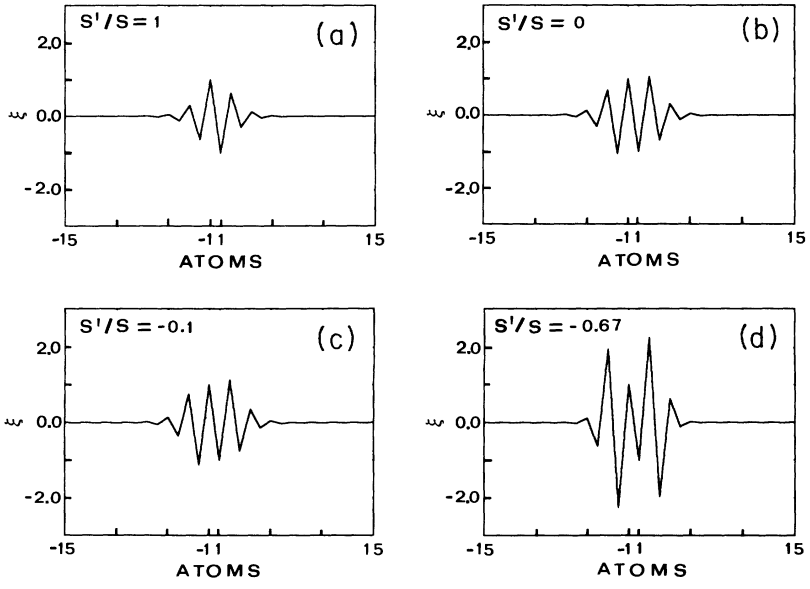

FIG. 6. Displacement pattern of even-parity modes for $S=0.1$ as a function of the force-constant ratio S'/S, as indicated in the legend of the panels.

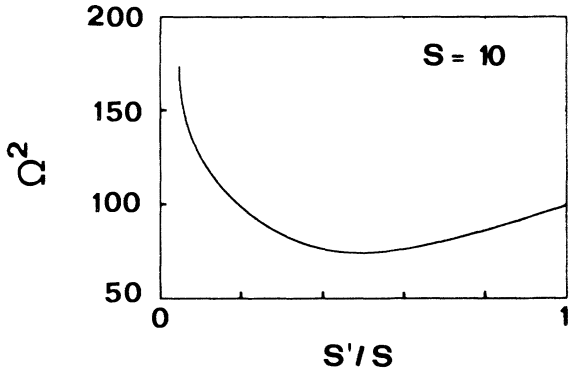

FIG. 7. Frequency squared of even-parity modes for $S=10$ as a function of the force-constant ratio S'/S.

ops the double-peaked structure with maximum displacement at $n=\pm 2$. Below this value of S'/S the solutions of Eq. (11) are no longer numerically stable, as happened in the previous case for the negative value of S'/S shown in Fig. 6(d). The displacement patterns for various values of S'/S are presented in Fig. 8. Large anharmonicity S produces a very narrow mode, involving six atoms only, so that the effect of the splitting produced by the local inhomogeneity appears less evident than in the previous case. We have performed similar calculations for the odd modes using a linear chain of 513 atoms, with an intrinsic localized mode centered at $n=0$, sketched in Fig. 9. The equations of motion to be solved in this case are the following, where we have chosen the normalization condition $\xi_0=1$:

$$
\begin{aligned}
&\Omega^2\xi_{-256}=(\xi_{-256}-\xi_{-255})+S[(\xi_{-256}-\xi_{-255})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-n}=(2\xi_{-n}-\xi_{-n+1}-\xi_{-n-1})+S[(\xi_{-n}-\xi_{-n+1})^3+(\xi_{-n}-\xi_{-n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-1}=(2\xi_{-1}-\xi_0-\xi_{-2})+S[(\xi_{-1}-\xi_{-2})^3+S'(\xi_{-1}-\xi_0)^3]\\
&\Omega^2\xi_0=(2\xi_0-\xi_{-1}-\xi_{+1})+S'(\xi_0-\xi_{-1})^3+S'(\xi_0-\xi_{+1})^3\\
&\Omega^2\xi_{+1}=(2\xi_{+1}-\xi_0-\xi_{+2})+S(\xi_{+1}-\xi_{+2})^3+S'(\xi_{+1}-\xi_0)^3\\
&\qquad\vdots\\
&\Omega^2\xi_{+n}=(2\xi_{+n}-\xi_{+n+1}-\xi_{+n-1})+S[(\xi_{+n}-\xi_{+n+1})^3+(\xi_{+n}-\xi_{+n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{+256}=(\xi_{+256}-\xi_{+255})+S[(\xi_{+256}-\xi_{+255})^3]\ .
\end{aligned}
\tag{12}
$$

The results are very similar to those of even modes. The only difference is that the value of S'/S at which the numerical instability of the solutions occurs is much larger than in the even case. This indicates that a small inhomogeneity is sufficient to produce the double-peaked structure. In Fig. 10 are presented the displacement patterns for various values of S'/S for $S=0.1$. In this case the numerical instability of the solution occurs at

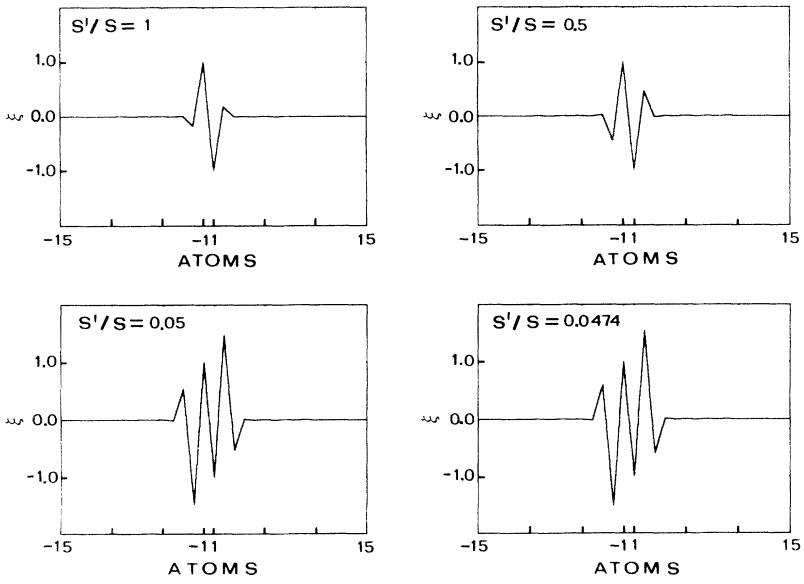

FIG. 8. Displacement pattern of even-parity modes for $S=10$ as a function of the force-constant ratio S'/S, as indicated in the legend of the panels.

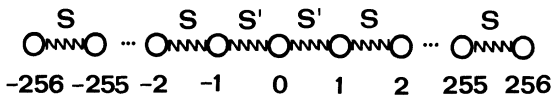

FIG. 9. Sketch of the anharmonic interactions in the free-end inhomogeneous one-dimensional chain of 513 atoms. S refers to unmodified force constants and S' to the modified force constant between the atom at the center of the chain and its nearest neighbors.

$S'/S=0.375\,75$. We have investigated the reason for this instability. We have found that below this value there are solutions with neighboring atoms moving in the same direction. This indicates that this mode arises from a harmonic mode different from the mode at the top of the harmonic band for which two neighboring atoms move out of phase: $\xi_{-n}=(-1)^n|\xi_{-n}|$. Lowering the ratio S'/S causes Ω^2 to decrease, and for $S'/S\leq -0.002$ the mode merges into the quasicontinuum of harmonic modes, becoming a broad resonance spread out over many atoms. In Fig. 11 is shown this new type of localized solution for $S'/S=0.006$ and in Fig. 12 is shown the broad resonance for $S'/S=-0.002$. From Fig. 11 one can see that the displacements of the neighboring atoms $n=+3$ and $n=+4$ are in the same direction, as well as for the atoms $n=-3$ and $n=-4$.

IV. INHOMOGENEOUS LINEAR CHAIN: ASYMMETRICAL LOCAL INHOMOGENEITY

In this section we present the results for the asymmetrical local inhomogeneity case, with the modified fourth-order anharmonicity parameter S' moved with respect to the center of the intrinsic localized mode, as shown schematically in Fig. 13 for the even modes. The equations of motions for this configuration are

$$
\begin{aligned}
&\Omega^2\xi_{-256}=(\xi_{-256}-\xi_{-255})+S[(\xi_{-256}-\xi_{-255})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-n}=(2\xi_{-n}-\xi_{-n+1}-\xi_{-n-1})+S[(\xi_{-n}-\xi_{-n+1})^3+(\xi_{-n}-\xi_{-n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{-2}=(2\xi_{-2}-\xi_{-1}-\xi_{-3})+S(\xi_{-2}-\xi_{-3})^3+S'(\xi_{-2}-\xi_{-1})^3\\
&\Omega^2\xi_{-1}=(2\xi_{-1}-\xi_{-2}-\xi_{+1})+S[(\xi_{-1}-\xi_{-2})^3+(\xi_{-1}-\xi_{+1})^3]\\
&\Omega^2\xi_{+1}=(2\xi_{+1}-\xi_{-1}-\xi_{+2})+S'(\xi_{+1}-\xi_{+2})^3+S(\xi_{+1}-\xi_{-1})^3\\
&\Omega^2\xi_{+2}=(2\xi_{+2}-\xi_{+1}-\xi_{+3})+S'(\xi_{+2}-\xi_{+1})^3+S(\xi_{+2}-\xi_{+3})^3\\
&\qquad\vdots\\
&\Omega^2\xi_{+n}=(2\xi_{+n}-\xi_{+n+1}-\xi_{+n-1})+S[(\xi_{+n}-\xi_{+n+1})^3+(\xi_{+n}-\xi_{+n-1})^3]\\
&\qquad\vdots\\
&\Omega^2\xi_{+256}=(\xi_{+256}-\xi_{+255})+S[(\xi_{+256}-\xi_{+255})^3]
\end{aligned}
\tag{13}
$$

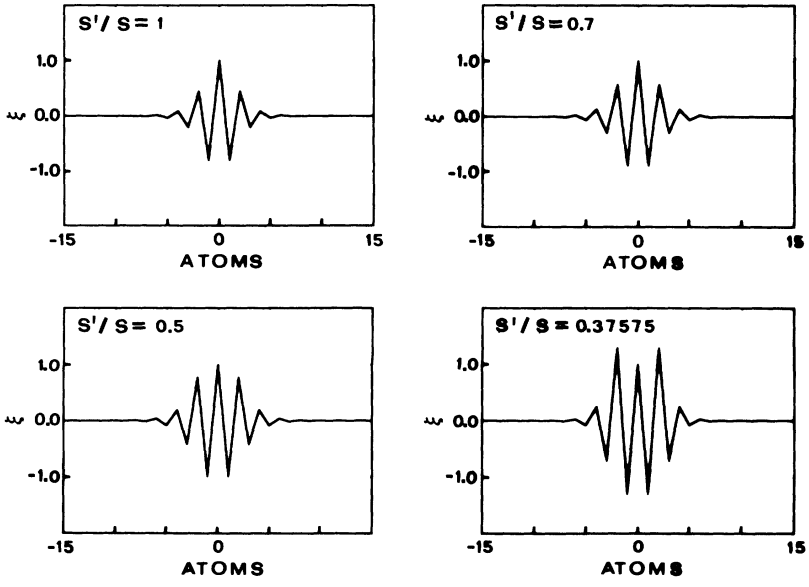

FIG. 10. Displacement pattern of odd-parity modes for $S=0.1$ as a function of the force-constant ratio S'/S, as indicated in the legend of the panels.

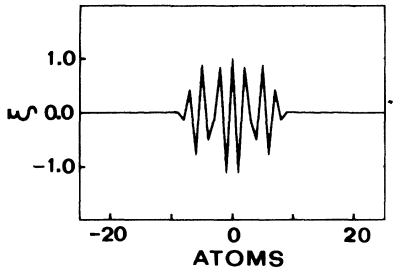

FIG. 11. Displacement pattern of the odd-parity localized mode for $S'/S=0.006$.

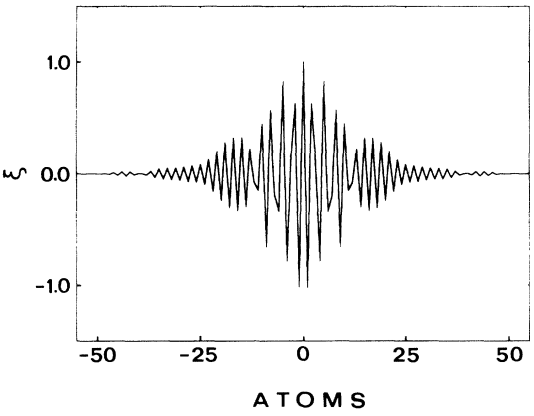

FIG. 12. Displacement pattern of the odd-parity resonance mode for $S'/S=-0.002$.

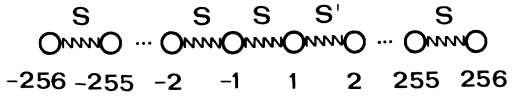

FIG. 13. Sketch of the anharmonic interactions in the free-end inhomogeneous one-dimensional chain of 512 atoms. S refers to unmodified force constants and S' to the modified force constant between the atoms $+1$ and $+2$ shifted with respect to the center of the chain.

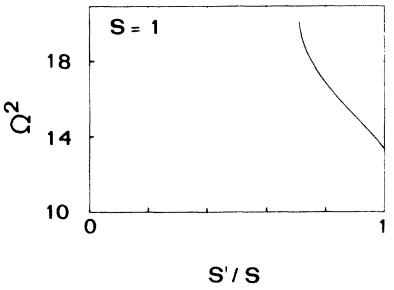

FIG. 14. Frequency squared of the asymmetrical inhomogeneous chain for $S=1$.

with the normalization condition $\xi_{-1}=1$. In Fig. 14, we plot Ω^2 as a function of S'/S for $S=+1$. There is a rapid increase of Ω^2 due to the large displacements acquired by the atoms at $n=+1$ and $n=+2$, as one can see in Fig. 15. The numerical instability of the solution for this configuration occurs at $S'/S=0.71$. It is important to note the breaking of symmetry in the displacement pattern between atom $n=+1$ and $n=-1$. The even mode tends to transform into an odd mode with its center on the atom $n=+1$. The symmetry reached by the mode is not exactly odd, because of the different couplings (S' and S) of the atom in $n=+1$ with left and right nearest neighbors. We have also investigated the configuration with local modification of the fourth-order anharmonicity between atom $n=+1$ and atom $n=+2$, but in this case the displacements pattern of the localized mode remains nearly unchanged because of the initial narrowness of the mode. The initial relative displacement of atom $n=+2$ is too small and cannot be enhanced significantly by decreasing the ratio S'/S.

V. SURFACE MODES

We have also studied the existence of localized modes close to the end atom of the finite chain with free ends. As in the previous sections we have used a 512-atom chain. The equations of motion that we have used are the same as in Sec. III with $S'=S$ and a different normalization condition. In this case we try to solve Eqs. (11) and (12) starting with an initial guess for the displacements that is always zero except on the last few atoms of the chain. In the case of the pure anharmonic interaction we have found the existence of a surface even mode and a surface mode similar to odd symmetry modes. The displacement patterns are reported in Table I for $\Omega^2=9.6$ in

TABLE I. Surface mode displacements. N indicates the end atom of the chain.

Atom	ξ_n (even mode)	ξ_n (quasiodd mode)
N	−0.165	0.614
$N-1$	1.000	−1.000
$N-2$	−1.000	0.394
$N-3$	0.166	−0.009
$N-4$	−0.0004	+0.0
$N-5$	+0.0	+0.0

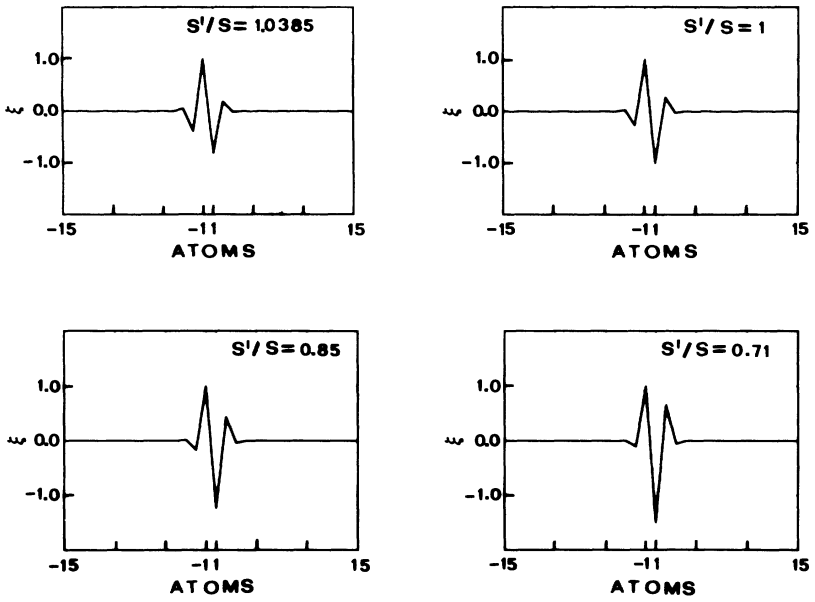

FIG. 15. Displacement pattern of even-parity modes of the asymmetrical inhomogeneous chain for $S=1$ as a function of the force-constant ratio S'/S, as indicated in the legend of the panels.

the even case and $\Omega^2=6.91$ in the quasiodd case. The frequency of these purely anharmonic surface modes scales with the maximum amplitude ξ_M so that all the infinite modes with Ω^2/ξ_M^2 constant are equivalent.

We have examined also the case of a chain with a weak harmonic interaction, such as $\frac{1}{10}$ of the quartic anharmonic interaction, and we have found that there is a shift in frequency and only a slight modification of the displacement patterns that does not destroy the symmetry found for the purely anharmonic case.

VI. CONCLUSIONS

In this work we have studied numerically the formation of localized modes in a linear chain by including a quartic anharmonic nearest-neighbor interaction. We have shown that these localized modes originate from the high-frequency mode of the harmonic linear chain and that a small anharmonicity is sufficient to produce a considerable narrowing of the displacement pattern. We have also investigated the role of crystal inhomogeneity, introducing a modification of the fourth order force constant between two neighboring atoms at the center of the localized mode, which could describe for example the epitaxial growth of a layer onto the surface of a film of the same material. We have found that a small weakening of this force constant tends to enlarge the displacement pattern, keeping the original location of the maximum displacement, while a large weakening tends to split the displacement maximum of the localized mode into two maxima, with one maximum located to the left and the other to the right of the initial maximum. The creation of these two maxima is favored for odd modes where a smaller weakening allows this splitting of the maximum of the intrinsic mode. We have also analyzed the asymmetric case, showing that by shifting the modified anharmonic force constant one site to the right there is a tendency of the even mode to become a quasiodd mode centered at that site. Finally, we have studied the existence of surface modes in the free-end chain finding an even symmetry mode and a quasiodd symmetry mode for the purely quartic anharmonic case.

ACKNOWLEDGMENTS

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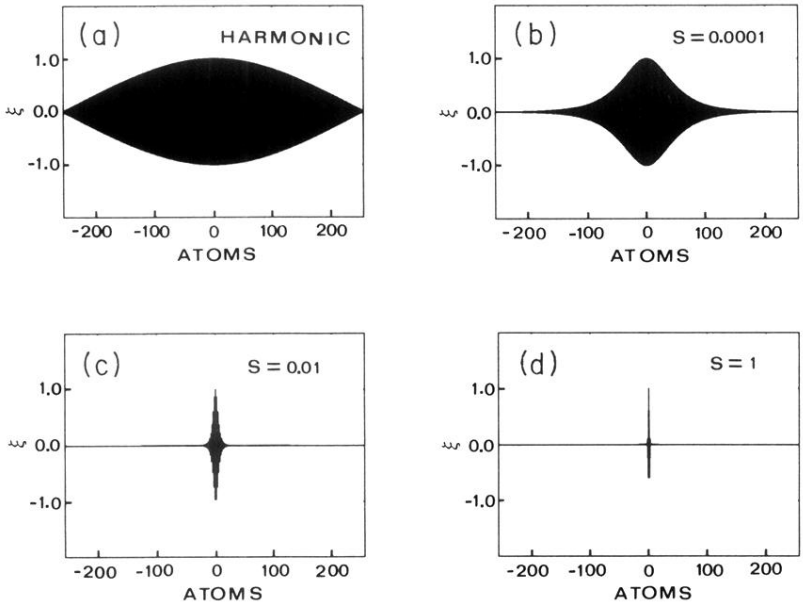

FIG. 1. Odd-parity localized modes. (a) shows the displacement pattern of the highest harmonic mode of a free-end one-dimensional chain of 513 atoms. For clarity the longitudinal displacements have been drawn vertically. (b) shows the odd localized mode of a chain with small anharmonicity ($S=0.0001$), (c) refers to the case $S=0.01$, and (d) to the case $S=1$.

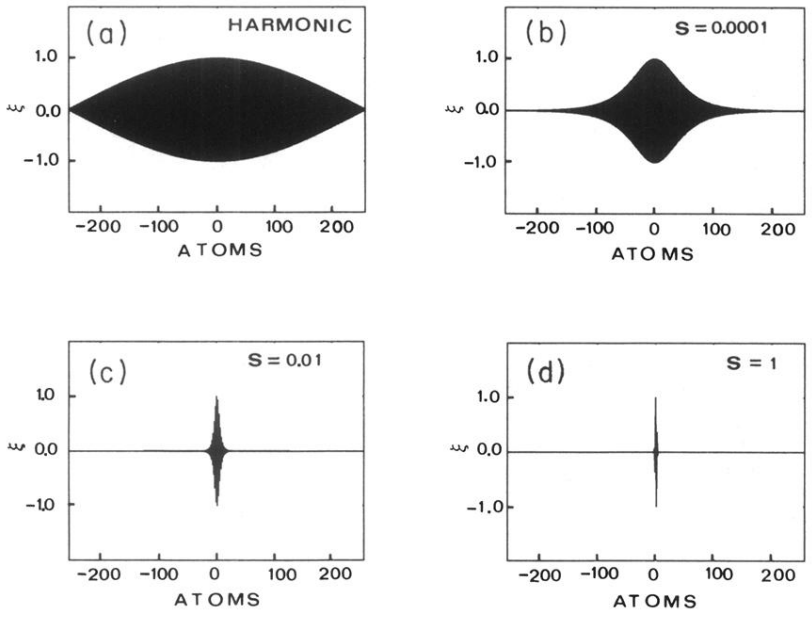

FIG. 2. Even-parity localized modes. (a) shows the displacement pattern of the highest harmonic mode of a free-end one-dimensional chain of 512 atoms. (b) shows the even localized mode of a chain with small anharmonicity ($S=0.0001$), (c) refers to the case $S=0.01$, and (d) to the case $S=1$.