Anharmonic localized surface vibrations in a scalar model

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(Received 15 December 1994)

Anharmonic excitations have been found and investigated that are localized at the surface of one-, two-, and three-dimensional lattices having simple cubic structure. A scalar model has been used with a single scalar degree of freedom per lattice point and short-range interactions. The nonlinear modes involve only a small number of particles or are extended along the surface. The stability of the nonlinear excitations has been analyzed and the nonlinear dynamics induced by an instability has been monitored by molecular dynamics.

I. INTRODUCTION

Anharmonicity of the interaction potential between particles in a crystal lattice can give rise to localized vibrations which, apart from a shift of its center, maintain their overall shape on long time scales. In integrable systems like the Toda lattice[1] and other integrable lattice models, these localized structures are solitons. In addition to moving solitons, stationary localized vibrating structures have been discovered[2–5] which resemble defect modes although the underlying lattice is homogeneous. In the integrable case of the Ablowitz-Ladik lattice,[6] such localized modes are a special case of lattice solitons. Recently, these localized modes have received a great deal of attention although there is no clear experimental evidence yet for their occurrence in real physical systems.

Systems which we regard as particularly promising for a successful experimental search for localized anharmonic vibrations are crystal surfaces and edges. This is because there are various experimental techniques to accommodate a high amount of energy locally on a surface and to analyze the resulting excitations. In addition, a large variety of adlayer structures exists with atoms of small masses which may be weakly bound to the substrate and therefore experience high vibrational amplitudes at given energy. Also, anharmonic vibrations near surfaces or edges bear additional interesting features as compared to their counterparts in the bulk. It has been shown by several authors[7–10] that localized anharmonic structures can occur as a result of modulational instability of a spatially extended nonlinear mode. The latter can be viewed as a nonlinear extension of Bloch-type phonon modes. If this nonlinear extended mode corresponds to a surface phonon mode, the nonlinear dynamics induced by the modulational instability is more complex than in the case of bulk phonons with energy being radiated into the bulk. The question then arises whether solutions of the equations of motion for the lattice degrees of freedom exist which are localized at the surface and involve only a few particles and whether such hot spots remain at the surface as a result of the instability of the extended surface state.

The investigations reported in this paper have been carried out on the basis of a scalar model which is natural in one dimension and has been applied for lattices in more than one dimension as well.[11,12] This means that to each lattice particle we attribute a scalar degree of freedom, which need not necessarily be interpreted as a particle displacement but could also play the role of a rotation angle in a molecular crystal, for example. For the interactions between the particles, the general distinction is made between systems having translational invariance and systems with nonlinear on-site potentials.

Anharmonic localized modes near the surface are presented for simple cubic lattices in one, two, and three dimensions. These solutions of the nonlinear equations of motion for the scalar degrees of freedom have been found by a search algorithm based on the rotating wave approximation. The solutions found in this way have been verified by molecular-dynamics simulations of the corresponding lattice, i.e., by a numerical integration of the equations of motion for the lattice degrees of freedom. A linear stability analysis has been performed for anharmonic surface modes analogous to the analysis of the stability of bulk modes by Sandusky *et al.*[13] The results of this stability analysis have again been verified by molecular-dynamics simulations. The interaction potentials assumed in these calculations include up to quartic anharmonic terms with the quartic term being positive (hard nonlinearity).

Recently, nonlinear surface waves in a simple cubic lattice within the scalar model have been investigated also for the case of soft nonlinearity, i.e., for a negative quartic term in the interaction potential.[12] Specifically, surface wave solutions have been found within the rotating wave approximation in the limits of long and short penetration depths. In the case of nearest-neighbor interactions only, these solutions have no linear limit. These earlier investigations have been extended to penetration depths of intermediate range, and the stability of such modes has been analyzed.

II. ANHARMONIC MODELS

The lattice-dynamical models considered in this investigation can be characterized by a Hamiltonian of the

form

$$H = \sum_{\ell} \frac{1}{2} p^2(\ell) + W(\{u(\ell')\}) \tag{2.1}$$

with the potential energy

$$W(\{u(\ell)\}) = \sum_{\ell} \Bigg\{ V(u(\ell)) + \frac{1}{2} \sum_{\ell' \epsilon N_\ell} \Bigg[\frac{K_2}{2} [u(\ell) - u(\ell')]^2 + \frac{K_3}{3} [u(\ell) - u(\ell')]^3 S(\ell, \ell') + \frac{K_4}{4} [u(\ell) - u(\ell')]^4 \Bigg] \Bigg\}. \tag{2.2}$$

A scalar degree of freedom $u(\ell)$ is attributed to each site ℓ of a semi-infinite simple cubic lattice in one, two, and three dimensions. For simplicity, we call these degrees of freedom displacements, although they may have different meanings depending on the physical system under consideration. $p(\ell)$ is the conjugate momentum of $u(\ell)$ and N_ℓ denotes the set of nearest neighbors of the site ℓ on the semi-infinite lattice. For the case of cubic anharmonicity, we have introduced the symbol $S(\ell, \ell') = 1$ if the nonzero component of the distance vector $\vec{R}(\ell) - \vec{R}(\ell')$ between sites ℓ and ℓ' is positive. Otherwise, $S(\ell, \ell') = -1$. Localized nonlinear surface vibrations will be studied in models including a nonlinear on-site potential $V(u)$, which is taken to be an even function of u, as well as models with translational invariance, i.e., $V = 0$.

III. SEARCH ALGORITHM FOR NONLINEAR LOCALIZED MODES

It is our aim to find time-periodic solutions of the equations of motion following from the Hamiltonian (2.1), which are localized at the surface of the underlying semi-infinite lattice. To achieve this, we apply the rotating wave approximation (RWA). The displacements $u(\ell)$ are expanded in a Fourier series

$$u(\ell, t) = \sum_{n=-L}^{L} U_n(\ell) e^{-in\omega t} \tag{3.1}$$

with $U_{-n}(\ell) = U_n^*(\ell)$, $L \to \infty$. This is inserted in the equations of motion. In equating to zero the sum of all terms proportional to $\exp(-i\omega t)$, we neglect the coupling to higher harmonics and obtain, in the absence of cubic anharmonicity,

$$\omega^2 U_1(\ell) = T(U_1(\ell)) + \sum_{\ell' \epsilon N_\ell} \Big\{ K_2 [U_1(\ell) - U_1(\ell')] + 3K_4 |U_1(\ell) - U_1(\ell')|^2 [U_1(\ell) - U_1(\ell')] \Big\} \tag{3.2}$$

with an on-site force $T(U(\ell))$ which can be formally written as

$$T(U) = \sum_{n=1}^{\infty} V^{(n)}(0) \frac{1}{n!(n-1)!} |U|^{2n} U. \tag{3.3}$$

The displacement amplitudes $U_1(\ell)$ are chosen to be real. In the presence of cubic anharmonicity (more general, of odd-order anharmonicity), the fundamental component in the expansion (3.1) of the displacements can couple to the static component $U_0(\ell)$. While the interaction of U_1 with higher harmonics is neglected, this latter coupling has to be accounted for in the presence of cubic anharmonicity.[13] This is accomplished by adding to the right-hand sides of (3.2) the term

$$\sum_{\ell' \epsilon N_\ell} \{ 2K_3 [U_1(\ell) - U_1(\ell')][U_0(\ell) - U_0(\ell')] S(\ell, \ell') + 3K_4 [U_1(\ell) - U_1(\ell')][U_0(\ell) - U_0(\ell')]^2 \} \tag{3.4}$$

and by supplementing (3.2) by the additional equation

$$0 = \sum_{\ell' \epsilon N_\ell} \big(K_2 [U_0(\ell) - U_0(\ell')] + K_3 \{ 2|U_1(\ell) - U_1(\ell')|^2 + [U_0(\ell) - U_0(\ell')]^2 \} S(\ell, \ell') + K_4 \{ 6|U_1(\ell) - U_1(\ell')|^2 + [U_0(\ell) - U_0(\ell')]^2 \} [U_0(\ell) - U_0(\ell')] \big) . \tag{3.5}$$

Cubic anharmonicity is considered here only in the case of translational invariance, i.e., $V = 0$.

Equations (3.2) with (3.4) and (3.5) are of the general form

$$\omega^2 U_1(\ell) = F_\ell(\{U_1(\ell'), U_0(\ell')\}) , \tag{3.6}$$

$$0 = G_\ell(\{U_1(\ell'), U_0(\ell')\}). \tag{3.7}$$

For the determination of solutions corresponding to localized vibrations, the following iterative search algorithm proved to be very efficient. It is outlined here for the case $K_3 = 0$. To simplify the notation, the index 1 at the variables $U_1(\ell)$ is suppressed, if cubic anharmonicity is absent.

The procedure starts with an initial guess for the displacement amplitudes $U^{(0)}(\ell)$ of the localized mode. Let ℓ_0 be the lattice site with the maximal displacement amplitude. From Eq. (3.6), the square of the initial frequency $\omega(0)$ is determined:

$$\omega^2(0) = F_{\ell_0}(\{U^{(0)}(\ell_0)\}) / U^{(0)}(\ell_0). \tag{3.8}$$

In the next step, new displacement amplitudes $U_1^{(1)}(\ell)$ are found via

$$U^{(1)}(\ell) = \alpha \omega^{-2}(0) F_\ell(\{U^{(0)}(\ell)\}) . \tag{3.9}$$

The scaling factor α is chosen such that $U^{(1)}(\ell_0) = U^{(0)}(\ell_0)$. In this way, the displacement amplitude of the site ℓ_0 is fixed to a given value. This procedure is iterated until convergence is reached. It has been extended to account for the static displacement amplitudes in the presence of cubic anharmonicity. In this case, the static displacements $U_0(\ell)$ have been determined in each step of the iteration by solving (3.7) for given $U_1(\ell)$. All localized solutions presented in the following sections have

been found with the help of this algorithm with certain modifications in some cases.

To verify the existence of the localized surface modes found in the framework of the RWA, a symplectic scheme[14] has been implemented for the numerical integration of the Hamiltonian equations resulting from (2.1) and (2.2). The initial conditions at time t_0 have been chosen as

$$u(\ell,t_0) = U_0(\ell) + 2U_1(\ell)\cos(\omega t_0)\ , \tag{3.10}$$

$$p(\ell,t_0) = -2U_1(\ell)\omega\sin(\omega t_0). \tag{3.11}$$

In all cases reported in the following (except for the situation discussed in Sec. VI), these numerical simulations confirmed the results obtained on the basis of the RWA. In particular, the power spectra for the displacements provided by the molecular-dynamics calculations show that higher harmonics are smaller by orders of magnitude.

IV. STABILITY ANALYSIS

To investigate the stability of nonlinear localized surface modes with respect to small perturbations of the displacements, we follow Sandusky *et al.*[13] and Sandusky *et al.*[10] and perform a linear stability analysis. The displacements $u(\ell)$ are decomposed into the localized surface mode solution, which we denote by $u_s(\ell)$, and a small deviation $\delta(\ell)$. Linearizing with respect to $\delta(\ell)$ yields

$$\ddot{\delta}(\ell) = -\sum_{\ell'} W_{\ell\ell'}\delta(\ell'), \tag{4.1}$$

where

$$W_{\ell\ell'} = \left.\frac{\partial^2 W(\{u(\ell)\})}{\partial u(\ell)\partial u(\ell')}\right|_{u(l)=u_s(l)} \tag{4.2}$$

are periodic functions of time with period $2\pi/\omega$.

The functions $W_{\ell\ell'}$ are expanded in a Fourier series

$$W_{\ell\ell'} = \sum_n W_{\ell\ell'}^{(n)} e^{-in\omega t} \tag{4.3}$$

with time-independent coefficients. They are computed from the representation (3.1) for the localized mode solution $u_s(\ell)$, confining ourselves to $L = 1$, i.e., to the RWA, except for the one-dimensional case, where the result of the RWA has been improved by taking up to five harmonics into account.

The Floquet theorem allows us to represent complex solutions for $\delta(\ell,t)$ in the form

$$\delta(\ell,t) = \sum_{n=-M}^{M} \Delta_n(\ell)e^{(\lambda-in\omega)t}. \tag{4.4}$$

The coefficients $\Delta_n(\ell)$ have to satisfy the following set of coupled equations:

$$(\lambda - in\omega)^2\Delta_n(\ell) = -\sum_{\ell'}\sum_{m=-M}^{M} W_{\ell\ell'}^{(n-m)}\Delta_m(\ell'). \tag{4.5}$$

It can be transformed into a non-Hermitian eigenvalue problem by introducing the additional variables $\Gamma_n(\ell) = \lambda\Delta_n(\ell)$. If the RWA [Eq. (3.10)] is used for the displacements $u_s(\ell)$ of the unperturbed mode, then $W_{\ell\ell'}^{(n)} = 0$ for $|n| > 2$ and the sum on the right-hand side of (4.5) contains only few terms. Furthermore, $W_{\ell\ell'}^{(-n)} = W_{\ell\ell'}^{(n)}$. If, in addition, $K_3 = 0$, then only $W_{\ell\ell'}^{(0)}$ and $W_{\ell\ell'}^{(-2)} = W_{\ell\ell'}^{(2)}$ can be nonzero.

The structure of (4.5) implies that if there is a solution with eigenvalue λ, there will be solutions with eigenvalues $-\lambda$ and λ^*, too. If λ' and λ'' are real and imaginary parts of an eigenvalue λ, and $\{\Delta_n(\ell)\}$ is an eigenvector corresponding to this eigenvalue, then

$$\delta(\ell,t) = e^{\lambda' t}\sum_{n=-M}^{M}\left[\Delta_n(\ell)e^{i(\lambda''-n\omega)t} + \text{c.c.}\right] \tag{4.6}$$

is a real solution of (4.1).

The nonlinear mode with displacements $u_s(\ell)$ is unstable if an eigenvalue λ occurs having a positive real part λ'. This real part of λ is called the growth rate λ_g of the corresponding perturbation of the nonlinear mode.

In the limit $M \to \infty$, the search for solutions of (4.5) with nonzero real part of λ would correspond to a full Floquet stability analysis equivalent to the one carried out by Sandusky *et al.*[10] for extended zone boundary modes in a nonlinear chain. In the absence of cubic anharmonicity, we confine ourselves here to $M = 1$. This corresponds to the assumption that an instability of a nonlinear mode of the form (3.1) sets in as a slowly growing perturbation of the amplitudes $U_{\pm1}(\ell)$. Our numerical simulations confirm this picture. For surface modes that are extended in the directions parallel to the surface in two and three dimensions, this procedure has to be modified by applying the Bloch-Floquet theorem for the spatial dependence of the eigenvectors parallel to the surface. In the one-dimensional case and for anharmonic modes localized in all spatial directions, the eigenvalue problem (4.5) can be solved for a finite lattice, if the instability eigenvectors are localized at the position of the anharmonic mode and do not extend too far into the substrate. This was found to be the case for $K_3 = 0$. The boundary conditions imposed on the truncation points of the lattice are then irrelevant if they are sufficiently distant from the position of the localized mode. However, in the presence of cubic anharmonicity and translational invariance in the one-dimensional case, eigenvectors have been found which extend far into the substrate. This situation is dealt with in the following way.

We label the lattice sites of the semi-infinite chain successively by $\ell = 0, 1, 2, \ldots$ with $\ell = 0$ denoting the tip site. Let ℓ_c be a lattice site sufficiently far away from the localized mode, such that $u_s(\ell_c) = 0$. For $\ell > \ell_c$ (4.5) simplifies to

$$(\lambda - in\omega)^2\Delta_n(\ell) = K_2[\Delta_n(\ell+1) + \Delta_n(\ell-1) - 2\Delta_n(\ell)], \tag{4.7}$$

which can be solved by the ansatz $\Delta_n(\ell) = \Delta_n(\ell_c) Z_n^{\ell-\ell_c}$. Here, Z_n is the solution of

$$(\lambda - in\omega)^2 = K_2(Z_n + Z_n^{-1} - 2) \tag{4.8}$$

having modulus smaller than 1. This precludes exponential growth of the eigenvector into the substrate. In Eq. (4.5), the index ℓ may now be restricted to run only from 0 to ℓ_c. The lattice sum on the right-hand side of (4.5) runs over site ℓ and its nearest neighbors with

$$\Delta_n(\ell_c + 1) = \Delta_n(\ell_c) Z_n. \tag{4.9}$$

In this way, the analysis is reduced to a finite lattice with a modified boundary condition at ℓ_c. Solutions of (4.5) with (4.9) have been determined numerically by a modified version of the inverse iteration scheme.[15]

When solving Eq. (4.5) without eliminating the quasiharmonic part of the eigenvector via (4.9), the results for the growth rate were found to depend strongly on the size of the lattice.

In all cases where instabilities have been found by the above method, the predicted maximal growth rate has been verified in a molecular-dynamics simulation by seeding the displacement pattern associated with the corresponding perturbation in the same way as done by Sandusky *et al.*[13] and Sandusky *et al.*[10] In the case of an instability with λ'' in the phonon frequency band, where (4.9) applies, the simulations have also been carried out for a finite lattice. However, damping has been introduced on lattice sites far away from the surface to suppress reflected waves.

V. MODELS WITH HARD NONLINEARITY AND TRANSLATIONAL INVARIANCE

In this section, nonlinear localized surface modes are discussed in models without on-site potential V. If, in addition, the coefficients K_2 and K_3 are zero, the frequency of a time-periodic solution scales with the displacement amplitudes. Applying this simple model to a semi-infinite chain, a mode has been found that is located near the end of the chain. However, the end atom is not the one with the maximal vibrational amplitude. Therefore, we do not regard it as a surface mode in the strict sense. The displacement pattern shown in Fig. 1 reveals that this mode is related to the antisymmetric bulk mode for the same model in an infinite chain discovered by Page.[5] As for the corresponding bulk mode, linear stability analysis as well as molecular dynamics show that this mode is stable. Including linear coupling ($K_2 \neq 0$) while keeping the maximal amplitude $U_{\max}$ constant causes the displacement pattern to be shifted further away from the end of the chain. Such modes localized near the end of a linear chain have also been reported earlier by ourselves[16] and also by Watanabe and Takeno[17] and by Wallis *et al.*[18]

If cubic anharmonicity is added, a pronounced static displacement is superimposed on the vibrations (see Fig. 2). The generation of static strains by cubic anharmonicity is well known for acoustic surface modes in the continuum limit[19,20] as well as for intrinsically localized lattice modes.[21,10] The Fourier spectrum for the displacement of the atom with maximal amplitude, as recorded in the molecular-dynamics simulation, is shown in Fig. 3 for the parameters $K_2 = K_3 = K_4 = 1$. As mentioned earlier, the contribution of higher harmonics, especially of even harmonics, is very small.

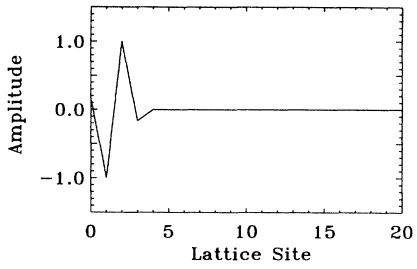

FIG. 1. Nonlinear surface mode in a semi-infinite chain with purely quartic interactions between neighboring sites.

Another interesting feature in the Fourier spectrum is a small peak in the phonon band. It corresponds to an instability of the intrinsically localized mode that has developed out of numerical noise or inaccuracy of the initial conditions. This instability has also been found in the stability analysis outlined in Sec. IV, making use of (4.7)–(4.9). The imaginary part λ'' of the eigenvalue λ is the frequency at which the small peak in the Fourier spectrum occurs. There are also pronounced side bands at frequencies $\omega \pm \lambda''$ and $3\omega \pm \lambda''$ as expected from the stability analysis. Since the value of λ'' lies in the band of linear phonon modes and the $\Delta_0(\ell)$ are nonzero, this instability generates radiation of energy into the bulk of the chain. At sufficiently large distances from the localized mode, the perturbation δ is of the approximate form

$$\delta(\ell, t) \sim e^{\lambda_g(t-\ell a/V)} e^{-i(\kappa \ell a - \lambda'')t} + \text{c.c.}, \tag{5.1}$$

where V is the group velocity and κ the wave number of linear lattice waves with frequency λ'' and a is the equilibrium lattice spacing. To obtain (5.1), use has been made of the fact that $\lambda_g \ll \lambda''$.

In order to confirm that this type of instability is not

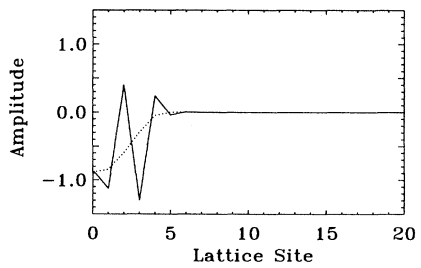

FIG. 2. Nonlinear surface mode in a semi-infinite chain with $K_2 = K_3 = K_4 = 1$.

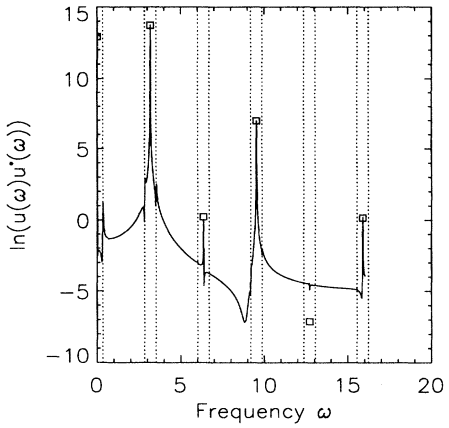

FIG. 3. Power spectrum for the displacement of the second lattice site of the mode shown in Fig. 2. The squares show the intensities for the Fourier components obtained by solving the equations of motion with $L = 5$. The dashed lines indicate the frequencies of the instability found by the stability analysis for the semi-infinite chain.

an artifact of the RWA, we have increased the number of harmonics L in the determination of the localized mode and M in the stability analysis. The results for the mode frequency and growth rate are shown in Table I. They suggest that harmonics beyond the third are irrelevant for this instability.

It was shown by Sandusky *et al.*[13] that a traveling nonlinear localized bulk mode in a chain with $K_3 = 0$ can be created by superimposing on the displacements of the (even) Takeno-Sievers mode[4] a small perturbation having odd symmetry. In this way, we let a nonlinear localized bulk mode travel from the interior of a semi-infinite chain to its end. It is found that the traveling mode is completely reflected and no trapping at the surface has been observed.

It has already been pointed out that the mode discussed above does not have its maximal displacement at the surface. From a numerical search in which the displacement amplitudes $U_1(\ell)$ are calculated in an iterative way from a given displacement amplitude at the surface at given frequency, we conclude that nonlinear surface modes with maximal displacements do not exist for the model with $K_2 = K_3 = 0$ in one dimension. The situation is completely different in two dimensions, where several modes with maximal displacements at the surface have been found. The displacement amplitudes of two modes ($S1, S2$) with symmetric and two modes ($A1, A2$) with antisymmetric character are given in Table II for the case $K_2 = K_3 = 0$. Modes $S2$ and $A2$ do not have their maximum amplitude at the surface. While the symmetric modes are stable, the antisymmetric modes are found to be unstable. However, the instability does not destroy these modes but causes them to oscillate between neighboring sites. This has been observed in molecular dynamics.

As harmonic coupling is included ($K_2 \neq 0$), the mode pattern shifts into the bulk of the lattice and becomes comparable to nonlinear bulk modes discovered by Fischer[22] in a two-dimensional lattice with $K_2 = 0$. For $K_4 U_{\max}^2 / K_2 = 1/4$, two modes were found with dis-

TABLE I. Dependence of the fundamental frequency on the number L of harmonics included in the calculation of the anharmonic surface mode with $K_2 = K_3 = K_4$. The maximum of $|U_1(\ell) - U_1(\ell+1)|$ is fixed. The dependence on M and L of real part (λ') and imaginary part (λ'') of the eigenvalue λ of the instability visible in the Fourier spectrum Fig. 3 is also shown.

L	ω	M	λ'/ω	λ''/ω
1	3.141	1	0.0026	0.1012
1		3	0.0024	0.0932
1		5	0.0024	0.0932
2	3.141	2	0.0025	0.1013
3	3.180	3	0.0027	0.1077
4	3.180	4	0.0027	0.1077
5	3.180	5	0.0027	0.1077

TABLE II. Displacement pattern and frequencies of surface localized modes. $K_2 = K_3 = 0$. The first column corresponds to the surface layer, the second column to the first sublayer, etc.

Mode $S1$, $\omega = 2.35\sqrt{K_4}U_{\max}$				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0049	0.0000	0.0000	0.0000	0.0000
-0.3251	0.0149	0.0000	0.0000	0.0000
1.0000	-0.3984	0.0092	0.0000	0.0000
-0.3251	0.0149	0.0000	0.0000	0.0000
0.0049	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000
Mode $S2$, $\omega = 2.44\sqrt{K_4}U_{\max}$				
0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	-0.0022	0.0000	0.0000	0.0000
-0.0044	0.2577	-0.0045	0.0000	0.0000
0.2514	-1.0000	0.2577	-0.0022	0.0000
-0.0044	0.2577	-0.0045	0.0000	0.0000
0.0000	-0.0022	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000
Mode $A1$, $\omega = 2.862\sqrt{K_4}U_{\max}$				
0.0002	0.0000	0.0000	0.0000	0.0000
-0.1338	0.0005	0.0000	0.0000	0.0000
1.0000	-0.1368	0.0002	0.0000	0.0000
-1.0000	0.1368	-0.0002	0.0000	0.0000
0.1338	-0.0005	0.0000	0.0000	0.0000
-0.0002	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000
Mode $A2$, $\omega = 3.020\sqrt{K_4}U_{\max}$				
0.0000	-0.0001	0.0000	0.0000	0.0000
-0.0002	0.1141	-0.0003	0.0000	0.0000
0.1152	-1.0000	0.1154	-0.0001	0.0000
-0.1152	1.0000	-0.1154	0.0001	0.0000
0.0002	-0.1141	0.0003	0.0000	0.0000
0.0000	0.0001	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000

TABLE III. Frequencies ω and maximal relative growth rates λ_g/ω of symmetric (S) and antisymmetric (A) bulk and surface modes for $K_2 = K_3 = 0$ (ω in units of $\sqrt{K_4}U_{\max}$).

	Bulk (S)		Bulk (A)		Surface (S)		Surface (A)	
Dimension	ω	λ_g/ω	ω	λ_g/ω	ω	λ_g/ω	ω	λ_g/ω
1	2.30	0.15	2.68	-			2.68	-
2	2.44	-	3.02	0.19	2.35	-	2.86	0.11
3	2.68	<0.01	3.29	0.25	2.55	-	3.16	0.23

placement patterns similar to $S2$ and $A2$. They are both unstable with growth rates $\lambda_g/\omega = 0.0029$ and $\lambda_g/\omega = 0.1287$, respectively. Modes of the type $S1$ and $A1$ have not been found with our search algorithm.

In the presence of cubic anharmonicity, static strains occur as is demonstrated in Fig. 4 for a nonlinear localized surface mode near a corner of the two-dimensional lattice.

At the surface of a three-dimensional simple cubic lattice, a number of nonlinear localized modes have been found in the pure quartic model (i.e., $K_2 = K_3 = 0$), including two unstable modes with symmetric displacement pattern and two stable modes with antisymmetric pattern. The displacement amplitudes of two modes in the first and second layer of the semi-infinite lattice are shown in Fig. 5. The displacements in the third layer are so small that they cannot be detected on the scale of the figure.

The second mode has the additional interesting feature that the bonds intersected by the dashed line are not involved in the dynamics. Hence it is possible to cut the lattice along these dashed lines to obtain a nonlinear mode localized at the corner of a three-dimensional lattice.

In Table III, frequencies and maximal growth rates of bulk and surface modes in one, two, and three dimensions are compared with each other for the following choice of parameters: $K_2 = K_3 = 0$, $K_4 = 1$, and $U_{\max} = 1/2$.

The effects of linear coupling on the modes in a 3D lattice are similar to those in a 2D lattice. In general, the displacement pattern is more localized with increasing number of nearest neighbors.

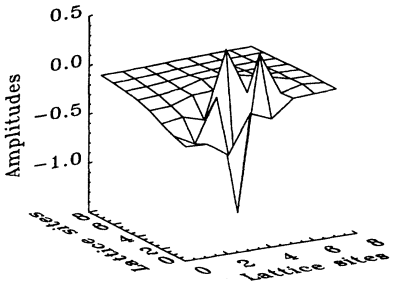

FIG. 4. Nonlinear surface mode in a two-dimensional lattice with $K_2 = K_3 = K_4 = 1$.

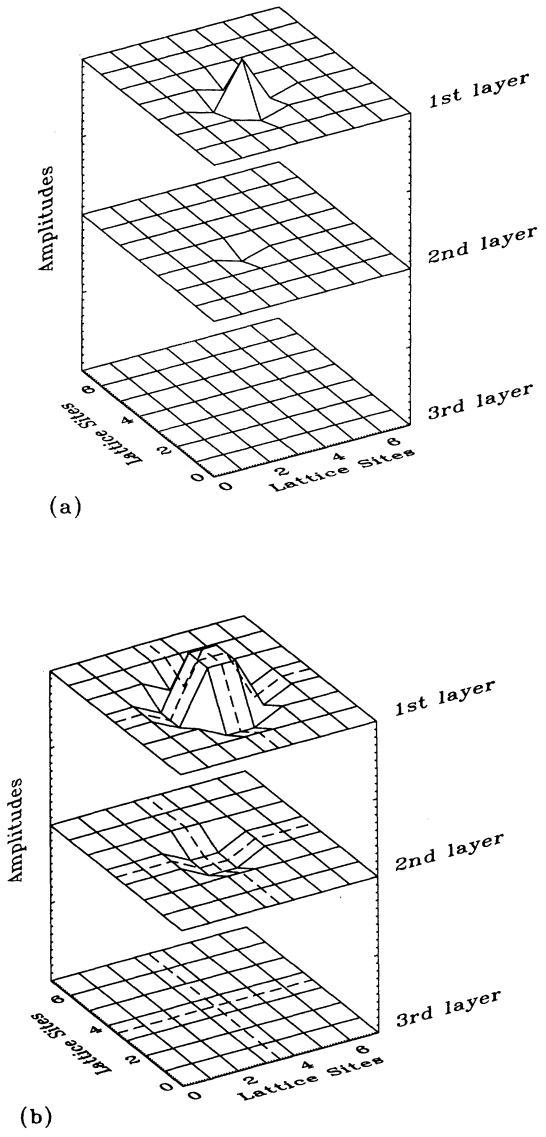

FIG. 5. Displacement patterns of two nonlinear surface modes (a) and (b) in a three-dimensional lattice with purely quartic interaction between nearest neighbors. The first three layers of the semi-infinite lattice are shown. The amplitudes $u(\ell)$ are visualized as out-of-plane displacements. Note that one can cut the lattice along the symmetry planes of the mode pattern (b) parallel to the crystal axes to obtain anharmonic corner modes.

VI. MODELS WITH SOFT NONLINEARITY AND TRANSLATIONAL INVARIANCE

A scalar model with harmonic and quartic anharmonic interactions between up to third neighbors in a semi-infinite simple cubic lattice has been considered by Kivshar and Syrkin,[12] who derived nonlinear surface modes within the RWA. Restricting the model to nearest-neighbor interactions only, its Hamiltonian becomes (2.1) with $V = 0$ and $K_3 = 0$. In this case, the nonlinear surface modes found by Kivshar and Syrkin have no linear limit. We confine ourselves here to this case. These surface modes are extended along the surface. Their displacement pattern is of the form

$$U(\ell) = f(R_3(\ell))e^{iq_1R_1(\ell)}e^{iq_2R_2(\ell)}, \tag{6.1}$$

where $\vec{R}(\ell)$ is the position vector of the lattice site ℓ and q_1 and q_2 are the components of a two-dimensional wave vector parallel to the surface. In the following, we set $q_2 = 0$ and disregard any dependence of the displacements on $R_2(\ell)$ to arrive at an effectively two-dimensional problem.

Two types of nonlinear surface modes of the form (6.1) have been found by Kivshar and Syrkin: those with very short penetration depth of only one lattice constant and those which penetrate deeply into the lattice. For both types, the case of soft nonlinearity, i.e., $K_4 < 0$, has been considered. The first type of mode is found to be highly unstable in the molecular-dynamics simulations due to the fact that the RWA is carried to the limit of its validity in this extreme case. The second type of mode has been found in the framework of continuum theory. More precisely, the profile function f is regarded as a continuous function of the argument $z = R_3$. Kivshar and Syrkin found the following expression for the profile function:

$$f(z) = \frac{\sqrt{2}Q}{\sqrt{h}\cosh[Q(z - z_0)]}, \tag{6.2}$$

where $h = -6\frac{K_4}{a^2K_2}[3 - 4\cos(q_1a) + \cos(2q_1a)]$ is a positive quantity. (a is the equilibrium nearest-neighbor distance.) The parameters Q and z_0 are related to each other via a boundary condition at the surface. Defining $\mu = Qz_0$, one obtains

$$Q = \frac{1}{a}\frac{\tanh(\mu)}{1 - 2/\cosh(\mu)^2} \tag{6.3}$$

and the nonlinear dispersion relation

$$\omega^2 = K_2[2 - 2\cos(q_1a) - a^2Q^2]. \tag{6.4}$$

These deeply penetrating modes can again be divided in two sets, one with maximum amplitude at the surface (set A) and one with maximum amplitude inside the bulk (set B). The iterative search procedure described in Sec. III has been extended by serial updating and taking a combination of the old and the new displacements. In this way solutions of the discrete system have been found which compare well with the continuum results by Kivshar and Syrkin. As had to be expected, they deviate from the continuum solutions for higher amplitudes and smaller penetration depths. In Fig. 6, the relations between frequency and amplitude for the continuum and discrete solutions are compared.

We examined the stability of the modes for q_1 at the boundary of the first Brillouin zone with respect to long-wavelength perturbations. The following ansatz has been made for the perturbation of the nonlinear mode solution:

$$\delta(\ell, t) = \exp\{i[q_1R_1(\ell) - \omega t]\}F(\ell, t) + \text{c.c.}, \tag{6.5}$$

where $F(\ell, t)$ is of the form

$$F(\ell, t) = \sum_{k\geq 0} P(R_3(\ell), t|k)\exp(ikR_1(\ell)) + Q^*(R_3(\ell), t|k)\exp(-ikR_1(\ell)). \tag{6.6}$$

Assuming exponential growth ($P(R_3(\ell), t|k)$, $Q(R_3(\ell), t|k) \sim e^{\lambda t}$) an eigenvalue problem for λ is obtained.

We found that the modes of both sets A and B are unstable. In Fig. 7, the maximal real part of the eigenvalues λ is plotted as a function of the maximum amplitude of the nonlinear mode and the wave number k of the perturbation. For the modes A, the growth rate is increasing with decreasing wavelength $2\pi/k$ of the perturbation. For the modes B there is a wavelength with maximal growth rate. By molecular dynamics, we confirmed our analysis and monitored the growth rate of the modes of set B. We were not able to confirm the growth rates of modes of set A, which may be due to the fact that the above stability analysis is valid only for long-wavelength perturbations. We observed the dynamics of the modes with seeded instability over a long time. It turns out that the mode patterns of both sets A and B are destroyed by the instability.

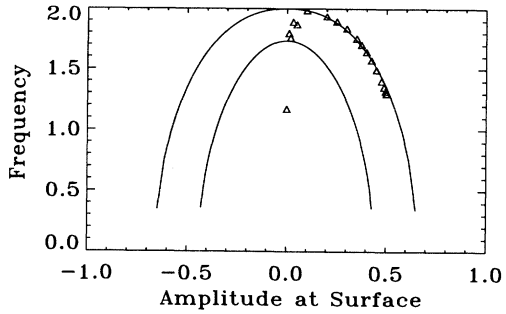

FIG. 6. Relation between frequency and amplitude of nonlinear extended surface modes in the model discussed in Sec. VI. Solid lines represent the continuum theory (Ref. 12). Triangles represent the lattice-dynamical calculation.

VII. ON-SITE NONLINEARITY

Scalar lattice models with nonlinear on-site potentials have been considered by several authors. Lee and Nasu[23] have studied a model with Hamiltonian of the form (2.1) and (2.2), where $K_3 = K_4 = 0$ and $V(u) = \frac{1}{2}\kappa_2 u^2 + \frac{1}{4}\kappa_4 u^4$. Applying the search routine described in Sec. III to a semi-infinite chain with this Hamiltonian, surface modes are obtained with maximum amplitude at the end of the chain, in contradistinction to the model with translational invariance, where such modes have not been found.

Pouget *et al.*[7] considered a sine-Gordon model with harmonic interaction between neighboring sites on a two-dimensional lattice. Here, the variables $u(\ell)$ have the physical meaning of orientational degrees of freedom. The intersite couplings were allowed to be anisotropic. In the isotropic limit, the corresponding Hamiltonian is given by (2.1) and (2.2) with $K_3 = 0$ and $V(u) = \kappa_0[1 - \cos(u)]$. (For $K_4 = 0$, this is the two-dimensional Frenkel-Kontorova model.) Pouget *et al.* demonstrated by numerical simulation how a spatially homogeneous nonlinear solution of the model decays into localized pulses as a consequence of modulational instability. Applying our search routine to this model (with $K_4 = 0$), solutions have been found which are localized at a free surface of the two-dimensional lattice (Fig. 8). The character of these surface modes is very different from corresponding solutions in models with translational invariance since in the latter, the scalar variable $u(\ell)$ of neighboring sites has opposite signs, i.e., the modes are of optic character, whereas the mode shown in Fig. 8 for the model with on-site nonlinearity is clearly of acoustic character.

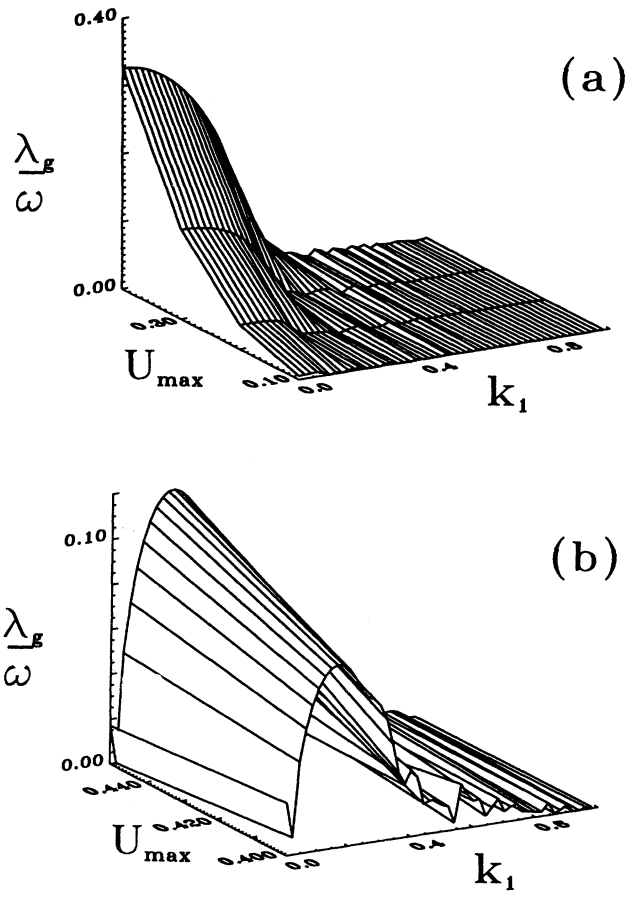

FIG. 7. Growth rate as function of wave number k_1 and maximal amplitude U_{max} of the nonlinear modes of Sec. VI. (a) refers to modes with maximum amplitude at the surface, (b) refers to the second type of surface modes.

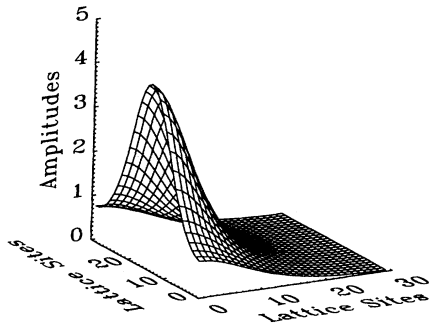

FIG. 8. Nonlinear localized surface mode of the sine-Gordon model with $\kappa_0 = 0.09$, $K_2 = 1$.

VIII. CONCLUSIONS

It has been shown for a scalar model by numerical search that various nonlinear localized modes exist at surfaces of simple cubic lattices in one, two, and three dimensions. The stability properties of these modes have been investigated, and different types of behavior have been found. Some modes proved to be stable, others are unstable, but the dynamics induced by the instability preserves the localization of the energy. In other cases, the instability leads to a complete destruction of the mode pattern.

The results reported in this paper all refer to a scalar model with one degree of freedom per lattice site. Nonlinear self-localized surface modes have also been found at the surface of a two-dimensional simple cubic lattice with the lattice particles having two-dimensional displacement vectors. These modes will be discussed in a forthcoming paper.

ACKNOWLEDGMENTS

It is a pleasure to thank J. B. Page, K. W. Sandusky, V. Bortolani, and A. Franchini for stimulating and helpful discussions. This work has been supported by the Deutsche Forschungsgemeinschaft through a grant and through the Graduiertenkolleg "Komplexität in Festkörpern: Phononen, Elektronen und Strukturen."

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