Ultrashort solitons in coupled electron-phonon systems

K. Hasenburg, E. Sigmund, and G. Mahler
Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 7000 Stuttgart 80, Federal Republic of Germany
(Received 10 February 1989; revised manuscript received 24 August 1989)

We numerically investigate the dynamical properties of a nonlinear quantum-mechanical model system of local electronic two-level centers coupled to acoustic phonons. Nonadiabatic processes are included. No rotating-wave approximation has been used. In spite of the discreteness of the lattice, "ultrashort" solitons are found with half-widths down to one wavelength of the phonons which are in resonance with the energy splitting of the two-level centers. In homogeneous systems solitons are created in pairs, while in heterosystems they may appear isolated. The solitons of a pair have different velocities, but the same half-width. We investigate the threshold behavior of the soliton formation and the stability of solitons against fluctuations. We perform numerical simulations of soliton-soliton and soliton-phonon interactions and discuss reflection processes at the end of the chain.

I. INTRODUCTION

The appearance of nonlinear excitations in anorganic structures as well as their possible formation in structured semiconductors is of increasing interest, especially for the development of new microelectronic devices.[1] In the area of self-induced transparency (SIT) it has been found experimentally and theoretically[2] that light pulses in resonance with the energy splitting of two-level centers embedded in a crystal may travel almost without any attenuation and retain a certain shape. However, in order to obtain such nonlinear effects sufficiently high light intensities are necessary. This is a disadvantage for the application in the field of information processing.

In this way the question arises of whether such a coherent pulse propagation may be possible in the case of phonons instead of photons. Aspects of this problem have already been investigated using a continuum approximation:[3] The underlying model in this case is an array of noninteracting, equidistant electronic two-level systems locally coupled to a lattice bearing acoustic phonons. A possible application of this model could be the transport of nonequilibrium acoustic phonons in insulating crystals with a high concentration of ionic two-level centers, as found, for example, in ruby.[4]

The main difference between the photon and phonon cases is obvious: While the typical photon wavelength extends over hundreds of two-level systems,[5] the wavelength of the "carrier phonons," i.e., those which are in resonance with the electronic center energy splitting, may well be of the same order as the typical distance between adjacent electronic centers. In order to draw conclusions about the stability of coherent excitations involving phonons with such a short wavelength, a number of commonly invoked approximations should be avoided: this applies to the mean-field approach as used in the SIT case, in which the centers are described in terms of a polarization density; instead, it is necessary to consider fluctuations caused by the discrete distribution of electronic centers. This is done in this paper by a direct numerical solution of the system of second-order differential equations of motion for the discrete model system.

In this approach, fluctuations are not regarded as a slight distortion of the soliton which can be taken into account by perturbation theory. The local basis allows us to directly take into account the whole phonon spectrum by which fluctuations are included without limitation automatically. Under certain circumstances this may lead to the decay of solitons which otherwise would be stable. Apart from fluctuations, for ultrashort pulses it is, of course, necessary to take into account the whole phonon spectrum, since the less extended the pulses are in real space the more extended they are in k space. Spontaneous decay is not considered.

Finally, we also avoid the rotating-wave approximation (RWA), where only the envelope of a given pulse is considered. Our numerical approach is applicable for any electron-phonon coupling constant. It makes it thus possible to investigate the properties and the stability of ultrashort pulses, which are defined by half-widths of the order of the resonant phonon wavelength (compare Ref. 6). In the numerical investigations it turns out that there exist solitons down to a half-width of about *one wavelength* of the carrier phonons: this corresponds to six lattice constants for the set of parameters chosen here and is remarkable because the solitons we describe are not topological, for they decay if the electronic and the vibrational excitations decouple. For information transport and processing, ultrashort pulses are of special importance in order to optimize (i) length scales and (ii) switching times.[7]

The concept of a soliton is introduced here from a rather practical point of view. In this paper a "soliton" is a nonlinear excitation of pulse shape that is stable over a period of time, some orders of magnitude larger than the decay time of resonant excitation pulses far below threshold. Their decay is generally caused by dispersion; in the present case the dispersion originating from the electron-

phonon coupling is much more important than the lattice dispersion, very similar to SIT, where dispersion clearly originates from the defect centers only. The term "pulse shape" refers here to the spatial dependence of the expectation value of local observables. Solitons in this sense may exist both in systems with translational invariance and in finite systems. In certain scattering processes they may lose small amounts (e.g., about 6%) of their energy and, if fluctuations are too strong, they even may decay. These are not solitons in the exact (idealized) meaning. Nevertheless, in this paper we will call these states solitons in order to stress their significance for a broader class of model systems, also. It should also be mentioned that SIT solitons lose energy in scattering processes in the case where different directions of motion relative to the lattice are considered.[8]

Our paper is organized as follows. After introducing the model Hamiltonian and the resulting equations of motion in Secs. II and III, we investigate the threshold behavior of the ultrashort-pulse dynamics in Sec. IV, which results in a hierarchy of fundamental excitations represented by phonons, breathers, and solitons. In Sec. V we discuss the nonlinear dynamics above soliton threshold and the coexistence of fundamental excitations. Our numerical approach with its direct solution of the second-order field equations allows a detailed investigation of the soliton stability during interaction processes where both directions of motion relative to the lattice are considered. This is presented in Sec. VI, together with a discussion of the stability against phonon interactions. Finally, in Sec. VII we turn to finite systems and investigate the reflection of ultrashort solitons from the end of the lattice.

Computer simulations can be regarded as "experiments," performed on model systems which may be defined by a set of differential equations, as in our case. Since initial values and parameters clearly have to be specified for each simulation, the method of deriving physical conclusions from numerical results is necessarily inductive. Determination of the range of parameters and initial conditions for the validity of our conclusions is very delicate because of the large state space of such a many-particle problem.

However, the results presented in this paper have been verified for a larger number of initial conditions and different combinations of coupling parameters. The diagrams presented in this paper only serve to exemplify the results.

II. MODEL HAMILTONIAN

In a local representation the system of noninteracting electronic two-level centers with the same energy splitting $\hbar\Omega$, which are locally coupled to a linear lattice bearing acoustic phonons, has the Hamiltonian

$$H=\sum_n \frac{1}{2M}p_n^2+\sum_n \tfrac{1}{2}D(u_{n+1}-u_n)^2+\hbar\Omega\sum_n (N_2)_n + \sum_n (u_{n+1}-u_n)(\hbar\lambda\sigma_n^+ +\hbar\lambda^*\sigma_n^-) , \tag{2.1}$$

where u_n and p_n are the displacement and momentum operators of the mass M at lattice site n, and D denotes the next-neighbor coupling.[9] The last term of Eq. (2.1) stands for the electron–acoustic-phonon interaction with the coupling constant λ. We have

$$(N_1)_n=(c_1^\dagger)_n(c_1)_n , \tag{2.2a}$$

$$(N_2)_n=(c_2^\dagger)_n(c_2)_n , \tag{2.2b}$$

$$\sigma_n^+=(c_2^\dagger)_n(c_1)_n , \tag{2.2c}$$

$$\sigma_n^-=(c_1^\dagger)_n(c_2)_n , \tag{2.2d}$$

the operators for the electronic system at lattice site n. $(c_1^\dagger)_n$, $(c_2^\dagger)_n$, $(c_1)_n$, and $(c_2)_n$ are Fermi creation and annihilation operators that act on the electron in the ground state (index 1) or in the excited state (index 2). $(N_1)_n$ and $(N_2)_n$ are occupation-number operators for the lower and upper level, respectively. $(N_1)_n$, $(N_2)_n$, σ_n^+ and σ_n^- obey the Pauli spin algebra commutator relations

$$[(N_2)_n,\sigma_n^\pm]=\pm\sigma_n^\pm , \tag{2.3a}$$

$$[\sigma_n^+,\sigma_n^-]=(N_2)_n-(N_1)_n , \tag{2.3b}$$

where σ_n^+ and σ_n^- play the role of the spin-flip operators. As the electronic centers do not interact directly, the electronic operators belonging to different elementary cells n commute.

III. EQUATIONS OF MOTION AND THE NUMERICAL PROCEDURE

The time evolution of the model system is obtained by Heisenberg's equation of motion

$$\dot{A}=\frac{i}{\hbar}[H,A] , \tag{3.1}$$

where A stands for the electronic and phonon operators, respectively. As the phonon operators and the electronic operators commute, we obtain the equations of motion

$$\ddot{u}_n=\frac{D}{M}(u_{n-1}-2u_n+u_{n+1})+\frac{\hbar}{M}[\lambda(\sigma_n^+-\sigma_{n-1}^+)+\text{H.c.}], \tag{3.2a}$$

$$\dot{\sigma}_n^+=i\Omega\sigma_n^+ +i(1-2(N_2)_n)\lambda^*(u_{n+1}-u_n) , \tag{3.2b}$$

$$(\dot{N}_2)_n=-i(u_{n+1}-u_n)(\lambda\sigma_n^+-\text{H.c.}) . \tag{3.2c}$$

In order to solve this coupled set of equations numerically, we proceed from the equations of operators to equations of expectation values.[10] These expectation values are the matrix elements of the operators taken over coherent states. This restriction is justified because in our model we consider coherent excitations in both the electronic and the vibrational systems. Furthermore, since we are interested in nonlinear effects, excitation energies are expected to be rather high. Thus the preconditions are given to confine ourselves to expectation values in a good approximation. We thus obtain

$$\ddot{u}_n=\frac{D}{M}(u_{n-1}-2u_n+u_{n+1})+\frac{2\hbar}{M}\text{Re}[\lambda(\sigma_n^+-\sigma_{n-1}^+)] , \tag{3.3a}$$

$$\dot{\sigma}_n^+ = i\Omega\sigma_n^+ + i(1-2(N_2)_n)\lambda^*(u_{n+1}-u_n) , \quad (3.3b)$$

$$(\dot{N}_2)_n = 2(u_{n+1}-u_n)\mathrm{Im}(\lambda\sigma_n^+) . \quad (3.3c)$$

Besides the bilinear product in Eq. (3.3c), the origin of the nonlinearity is the factor $1-2(N_2)_n$ in Eq. (3.3b) which arises from the Fermi commutation relation of the electronic operators. This is a pure quantum-mechanical effect. The coupling to Fermi systems can introduce nonlinear effects because if such a two-level system is excited to inversion [i.e., $(N_2)_n=1$], it is saturated and cannot accept any further excitation energy, i.e., the "spring" that transfers energy to the system has softened. If the factor $1-2(N_2)_n$ was dropped, the system would no longer lead to solitons.

Equations (3.3) are numerically integrated with periodic boundary conditions for systems of 300 and 600 lattice sites, respectively. An adequate algorithm to solve this problem is the combined prediction-correction multistep procedure of Adams, Bashford, and Moulton,[11] with a local error of order $O(h^6)$, where h is the iteration time step. This algorithm is very stable for the system of Eqs. (3.3) and the range of parameters investigated here. The convergence of the procedure is always checked very carefully by testing the local error of the local variables u_n, σ_n^+, and $(N_2)_n$. To adjust the iteration time step h, it also turned out to be very useful to calculate the expectation value of the total energy E_{tot}, which is very sensitive to numerical errors. E_{tot} was allowed to deviate by less than 1%. The stability of the algorithm is illustrated by the fact that even after a peak deviation amounting to 1%, e.g., in *all* the simulations the deviation of E_{tot} and the local error of the local variables again reduced below 0.1%, where it stayed approximately constant.

In this paper we apply the "natural" unit system (us), in which lengths are measured in units of the lattice constant a, the mass in units of the mass M of one elementary cell, and velocities in units of $c/2$ (where c is the sound velocity for $k=0$). Consequently, with $a_{\mathrm{us}}=1$, $M_{\mathrm{us}}=1$, and $c_{\mathrm{us}}=2$ in this unit system we obtain $D_{\mathrm{us}}=4$. The energy unit e.u. is given by 1 e.u.$=M(c/2)^2$ and the time unit t.u. by 1 t.u.$=2a/c$. Planck's constant is then $\hbar_{\mathrm{us}}=\hbar/(\text{e.u.}\times\text{t.u.})$. The actual numerical calculations are performed for $\hbar_{\mathrm{us}}=1$. A concrete physical application with $\hbar_{\mathrm{us}}\neq 1$ necessitates the rescaling $\lambda'=\hbar_{\mathrm{us}}^{-1/2}\lambda$ and $u_n'=\hbar_{\mathrm{us}}^{1/2}u_n$.

IV. FUNDAMENTAL EXCITATIONS

In most of the simulations we assume, as an initial condition, a running phonon wave packet

$$u_n(t=0)=u_0\mathrm{sech}[(n-n_0)/\Delta]\cos k_0 n , \quad (4.1)$$

with the carrier phonon wave number $k_0=\pi/3$ and a sech-type envelope of maximum value u_0, while $(N_2)_n=\sigma_n^+=0$ at all sites n. The parameters n_0 and Δ denote position and width of the phonon pulse, respectively. With $k_0=\pi/3$ the resonance condition for the coupled system is fulfilled for $D=4$, $M=1$, and $\Omega=2$. If the physical realization requires $\Omega\neq 2$, k_0 has to be adjusted appropriately. This, however, has no substantial influence on the physical results presented in the following sections, provided that k_0 is not so large that lattice-dispersion effects become too strong for soliton formation.

Extensive numerical studies have shown a significant difference between the time evolutions for the cases $\Delta\geq\Delta_{\mathrm{ch}}=4$ and $\Delta<\Delta_{\mathrm{ch}}$.[12] For the case $\Delta\geq\Delta_{\mathrm{ch}}$, the hierarchy of fundamental excitations is illustrated in Fig. 1 for $\Delta=8$ and electron-phonon coupling constant $\lambda=0.5$. The only difference between Figs. 1(a)–1(c) is the initial phonon amplitude u_0 which ranges from $u_0=0.21$ to $u_0=1.176$. The case $\Delta<\Delta_{\mathrm{ch}}$ will be discussed subsequently.

For small amplitudes [Fig. 1(a)] the phonon pulse is completely blurred over the whole system, as expected. In a first step, the initial phonon pulse, while moving to larger n, is completely absorbed by the electronic centers. However, although the electronic centers are only very slightly excited [i.e., expectation value $(N_2)_n<0.04$], the tail of the fading phonon pulse stimulates the electronic centers to reemit energy into the phonon system, by which a new, though retarded and broadened, phonon pulse is built up. In this way the excitation width continuously increases [see Fig. 1(a), $t=150$] and finally extends over the whole lattice. However, because of $(N_2)_n\ll 1$ [i.e., the factor $1-2(N_2)_n$ in (3.3) could be replaced by unity] this is not a nonlinear effect: The small-amplitude excitations of this type are therefore called "linear excitations" or sometimes "phonons" in this paper, although, strictly speaking, they are coupled excitations of the vibrational and the electronic system (compare the phonons in Ref. 13). In contrast to these linear excitations, solitons and breathers are nonlinear excitations.

An essential feature of the dynamics is the energy transfer between the electronic and the vibrational subsystem. The vibrational system is responsible for the transport of the excitation and the electronic system for its localization. This shows that even for weak (i.e., linear) excitations nonadiabatic processes are most important to describe the dynamical behavior adequately: Although the electronic excitation energy is yet very small, nonadiabatic processes are responsible for the blurring effect.

For larger excitation energies (i.e., increasing u_0) the nonlinear term $1-2(N_2)_n$ of Eq. (3.3b) becomes important [see Fig. 1(b)]. Because of this nonlinearity the localizing influence of the electronic centers produces a one-dimensional "self-focusing" effect [compare Fig. 1(b), $t=180$ to Fig. 1(a), $t=150$]. Despite complete inversion [see Fig. 1(b), $t=9$) and although the total energy is larger than the energy of a single slow soliton, we are still below the threshold and no solitons are formed. Comprehensive numerical studies show that for this type of initial condition [phonon pulse in homogeneous system, $(N_2)_n(t=0)=0$] only pairs of solitons are formed, and the minimum energy—threshold energy E_t—for such a pair (which is dependent on the initial pulse width Δ, see below) is not yet obtained.

Below soliton threshold the excitation does not yet

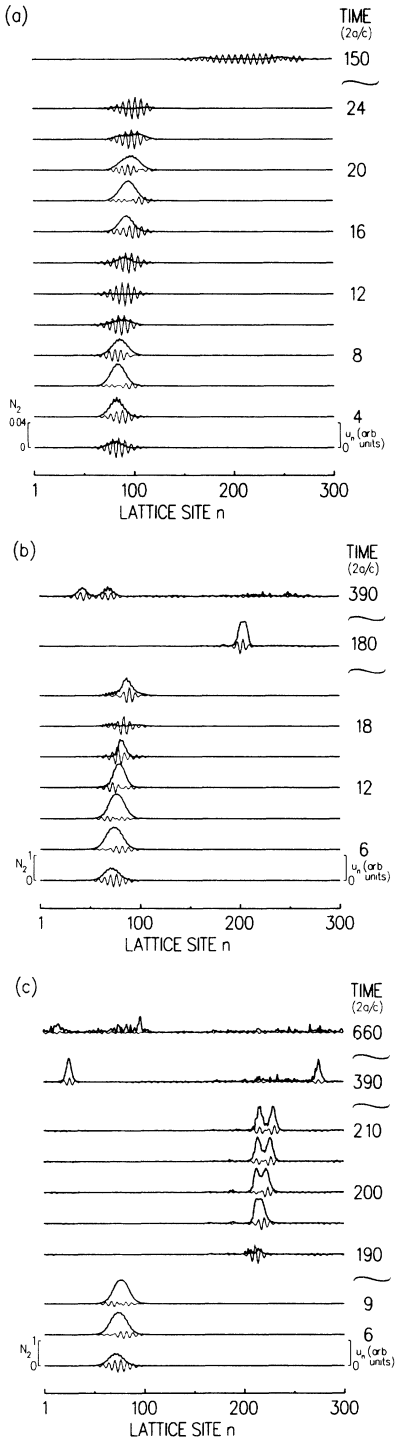

FIG. 1. Displacement u_n (thin line) and occupation number $(N_2)_n$ (heavy line) of the upper electronic level at site n, for a lattice of 300 sites. The time steps t and the electron-phonon coupling constant $\lambda=0.5$ are measured in the units defined in the text. The initial condition is a resonant sech-type phonon pulse [see Eq. (4.1)] with $\Delta=8$. $(N_2)_n=\sigma_n^+=0$ for all n. The initial maximum amplitudes are (a) $u_0=0.21$, resulting in a linear excitation; (b) $u_0=1.175$, a breather excitation finally splitting into two pulses without inversion; (c) $u_0=1.176$, the threshold case. Breather excitation, decomposing into two ultrashort solitons, which finally decay into decoupled vibronic and electronic excitations.

split up into solitons, but, rather, periodically changes its shape and transfers energy between the vibrational and the electronic system. Such an oscillation is depicted in Fig. 1(b), $t=3-18$. We call this excitation type "breather," corresponding to the same type of solution in SIT.[5] In contrast to the "linear excitation" the breather is self-focused and does not blur over the whole system [Fig. 1(b), $t=180$]. Similar to the SIT case, complete inversion is not necessary for breather dynamics. However, the "ultrashort breather" discussed in this paper is not as stable as a SIT breather. The long-time evolution reveals a dynamical behavior which significantly differs from the SIT case. The breather finally [for the simulation in Fig. 1(b) after $t=285$] splits into two stable pulses [see Fig. 1(b), $t=390$], which do not reach complete inversion $[(N_2)_{\max}=0.4]$. In the further time evolution the two pulses completely separate. Methods to analyze these excitations are being developed at the moment and are planned to be presented in a forthcoming publication.

In the breather regime, varying u_0 does not lead to an accordingly varying amplitude of the two pulses that result from the breather decay. Their respective amplitudes do not considerably exceed $(N_2)_{\max}=0.5$. For the given parameters, $\lambda=0.5$ and $\Delta=8$, this behavior drastically changes for $u_0\geq(u_0)_t=1.176$, the threshold phonon amplitude (with related threshold energy $E_t=44.37$, see Table I) . Here the electronic amplitude of the two resulting pulses abruptly jumps to $(N_2)_{\max}=1$. The threshold case is depicted in Fig. 1(c) [compare Fig. 1(c), $t=390$ to Fig. 1(b), $t=390$]. The small variation of initial amplitude from $u_0=1.175$ [Fig. 1(b)] to $u_0=1.176$ [Fig. 1(c)] yields for small t a correspondingly similar time evolution of breather oscillations [see Figs. 1(b) and 1(c), $t=3-9$], whereas for large t [see $t=390$ in Figs. 1(b) and 1(c)] there is a qualitative change. In Fig. 1(c), the breather finally decomposes ($t=190-210$) into two ultrashort solitons (see $t=390$). The half-width of the solitons amounts to little more than one wavelength of the resonant phonons, i.e., the solitons here are orders of magnitude narrower than those of SIT.

Contrary to both the phonon and the breather excitations, the processes of absorption and induced emission, which before acted on different phonon pulses, now act on the leading edge and the tail of the *same* phonon pulse inside the soliton, with the result that there are no more

TABLE I. Numerical results for the threshold amplitude $(u_0)_t$ and energy E_t for different initial phonon pulse widths Δ, for a system specified by $\lambda=0.5$, $D=4$, $M=1$. The units are defined at the end of Sec. III.

Δ (a)	$(u_0)_t$ (a)	E_t (e.u.)
2	3.00	75
4	1.89	58
4.5	1.70	52
6	1.422	49
8	1.176	44
12	1.025	50
16	0.975	61

breather oscillations, but there are stable pulse shapes for both the electronic and the vibrational excitations. There is now a metastable equilibrium of absorption and induced emission processes. The soliton half-width is much smaller than that of the initial phonon pulse. This type of "acoustical pulse compression" is very similar to the case in nonlinear optics.[5]

Finally, the solitons decay into localized electronic excitations and decoupled phonons [see Fig. 1(c), $t=660$]. This is not due to the discreteness of the lattice, as one might assume, but to fluctuations induced by those phonons, which are not bound to solitons but have been formed besides the solitons as a sort of "background excitation." The interaction of such phonons with a soliton may decouple the soliton's electronic part from its vibronic part. This will be discussed in Sec. VI [see, e.g., Fig. 6(b) for the analogous case of destructive soliton-soliton scattering]. The soliton instability increases with decreasing soliton half-width. Figure 2 [same initial condition as in Fig. 1(c), but system size $N=600$] shows that the smaller the phonon concentration the larger is the soliton lifetime. Here, the slower soliton decays after $t=780$ and the fast one not before $t=1300$. Preceding the decay, the solitons become decelerated. For the slower soliton this can readily be seen in Fig. 2 (beginning at $t=480$). However, the dynamical stability against disturbances is seen in Fig. 2, where the slower soliton recovers its original shape after the fluctuation at $t=600$.

Important questions concern (i) the universality of the threshold energy for soliton-pair formation, E_t [i.e., how E_t depends on initial conditions—in our case on envelope type (sech, Gaussian, etc.) and width Δ of the initial phonon pulse], and (ii) for which range of initial condition parameters soliton formation is possible at all. Table I comprises the results for $(u_0)_t$ and E_t of several series of computer simulations for sech-type initial phonon pulses with different Δ ($\lambda=0.5$, $D=4$, $M=1$). Other pulse shapes (e.g., Gaussian or box shape) do not give rise to substantial changes, except for a larger phonon background which raises E_t.

Soliton formation is possible for a broad range of Δ:

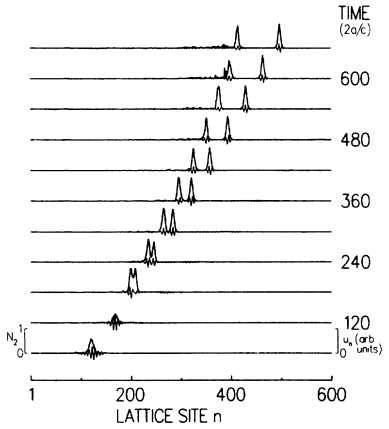

FIG. 2. Same as Fig. 1(c) ($u_0=1.176$, $\Delta=8$), but with 600 lattice sites: the two ultrashort solitons are more stable.

For $\lambda=0.5$ the lower limit is $\Delta=1$; below this value, dispersion effects become too strong. There appears to be no upper limit (simulations have been performed for $\Delta=40$ and 60), provided that the system size is at least about 1 order of magnitude larger than Δ so that the different excitations may develop and separate well.

The threshold energy E_t depends (i) on the total energy of the formed soliton pair (depending on Δ, the solitons have different velocities at the threshold), and (ii) on the total energy of the phonon background formed besides the soliton pair. The smallest E_t is obtained for $\Delta=8$ (see Table I), which is the value chosen for Figs. 1 and 2. Thus E_t is not universal. Universal, i.e., independent of initial conditions, is only the relation between the single soliton's total energy, its velocity, and half-width. This has been shown both numerically and analytically, the latter with the approximations commonly applied in SIT, but is not presented in this paper.

Depending on Δ we can distinguish between two significantly different soliton-formation processes (explicit numerical values are given for $\lambda=0.5$, $D=4$, and $M=1$): In the simulations with $\Delta\geq\Delta_{ch}=4$, the dynamic processes follow in principle the evolution depicted in Figs. 1(a)–1(c), with a hierarchy of phonons, breathers, and, for $E=E_t$, a breather state which finally divides into two solitons. For $\Delta<\Delta_{ch}$ there is no distinct hierarchy of phonons and breathers (besides a certain phonon background which is formed in general). For any u_0 the initial excitation at once divides into two stable pulses, which are similar to those formed after breather decay for $\Delta\geq\Delta_{ch}$. However, while for $\Delta\geq\Delta_{ch}$ the electronic excitation discontinuously jumps from $(N_2)_{max}\approx 0.5$ to 1 for $E=E_t$, for $\Delta<\Delta_{ch}$ the inversion continuously increases for increasing u_0, until—for $E=E_t$—complete inversion is obtained and thereby solitons are formed.

Thus we can define Δ_{ch} as the threshold width, where the character of nonlinear dynamics significantly changes from continuous ($\Delta<\Delta_{ch}$) to discontinuous ($\Delta\geq\Delta_{ch}$) behavior at the energy threshold E_t. For very broad initial phonon pulses ($\Delta>20$) the additional excitations formed besides the soliton pair (for $E\geq E_t$) become so strong that they induce nonlinear processes by themselves, which may result in the formation of further breather and soliton pairs. As mentioned above, for such simulations ($\Delta=40$ and 60) the system has to be chosen large enough ($N=900$), so that the breather and soliton pairs can separate properly.

The formation of such soliton pairs in homogeneous systems with periodic boundary conditions reminds one of topological kink-antikink sine-Gordon solitons. Indeed the equations of motion for the system of exactly resonant electronic centers considered here can be transformed to a sine-Gordon equation if the RWA and continuum approximation are applied,[5] together with some other approximations like the neglect of both the Doppler broadening and the phase variation of the phonons. However, it is remarkable that soliton formation can be shown at all, and even for such narrow nontopological solitons as described in this paper, where the preconditions for the validity of most of these approximations are heavily violated.[6] Two significant differences to

the sine-Gordon case, (i) the localization of phonons around fast solitons and (ii) the possible soliton decay in scattering processes, will be described in Secs. V and VI.

Up to now we have discussed soliton formation in homogeneous systems. However, both from theoretical and experimental points of view it is interesting to study soliton formation in structured systems. Indeed, it is possible to form single solitons without any background excitation, if a system geometry is chosen where the initial phonon pulse starts from a region A without electronic centers and then enters a region B with electron-phonon coupling (cf. Fig. 3 with $\lambda=0.2$, $D=4$, $M=1$). It should be mentioned that in all the computer simulations performed no reflection of the input phonon pulse is seen, independent of whether the phonon pulse shape is of sech, Gaussian, or step-function type. The whole input energy is transferred through the interface. Depending on the pulse envelope, zero, one, or more solitons with or without phonons and breathers is (are) formed. It turns out that single solitons, without background, are formed if the input phonon pulse has a sech-type envelope and satisfies certain requirements concerning u_0 and Δ: u_0 must equal the maximum amplitude u_s of the phonon part of the formed soliton. It is easily seen that then the width Δ' of the incident pulse has to be chosen c/v_s times the width Δ_s of the phonon part inside the soliton. Here v_s is the soliton velocity and c the group velocity of the incident phonon pulse. Only solitons with $v_s \leq c$ are found. For decreasing u_0, i.e., decreasing soliton energy, v_s becomes very small compared to c [cf. the slow soliton in Fig. 4(d)]. The simulations show that as a consequence Δ_s is much smaller than Δ'. Again, this effect could be called "acoustical pulse compression," but now it is occurring in a heterosystem. In our system, where dissipation effects are neglected, there is no lower limit for u_0, i.e., no upper limit for Δ'. This shows that at interfaces it is possible to form solitons from an incident phonon pulse, with an amplitude considerably too small for soliton formation in homogeneous systems [cf. Fig. 1(a)]: At interfaces even a small-amplitude excitation is able to induce nonlinear effects as the whole phonon pulse passes the electronic centers directly at the interface unattenuated, and its effect on these centers is integrated over time, thus producing inversion. In the homogeneous case, on the other hand, every part of the extended phonon pulse excites another electronic center, so that the pulse has been absorbed long before inversion could be reached. Clearly, in reality, dissipation effects will define an upper limit for the time over which very slow solitons can be formed.

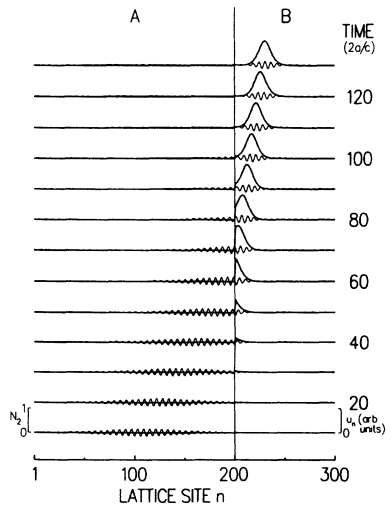

FIG. 3. Heterostructure with $\lambda=0$ in region A and $\lambda=0.2$ in region B. The initial condition is a resonant sech-type phonon pulse in region A with maximum amplitude $u_0=0.55$.

We have seen that for given u_0 there exists a pulse width Δ' where the phonon pulse does not change its amplitude while passing the interface, i.e., it is only compressed during soliton formation. It is interesting that Δ may vary inside a certain range around Δ', and yet single solitons are formed without background. In such a case the resulting phonon amplitude inside the soliton is smaller ($\Delta<\Delta'$) or larger ($\Delta>\Delta'$) than u_0. This range will be called the "soliton window," but will not be determined numerically in this paper. If Δ is outside the soliton window, either only phonons or breathers are formed (for small Δ) or a soliton plus background is produced (for large Δ). If, in the latter case, Δ is further increased, a second soliton window is entered, where two solitons without background are formed: Increasing Δ subsequently opens energetically equidistant soliton windows. This is an analogy to the area theorem of SIT.[2,5] In such a way it is possible to build up from an incoming plane wave a train of solitons nearly without any background excitation, where the velocity, width, and energy content of each soliton is the same and determined by the amplitude of the incident wave.

For pulse shapes other than sech type (e.g., Gaussian or box shape), the simulations performed always show the formation of a certain amount of background excitation. Clearly in this case only the lower limit of each soliton window can be determined precisely: This is the smallest Δ where one (two, three, . . .) soliton(s) are formed, respectively.

V. COEXISTENCE OF FUNDAMENTAL EXCITATIONS

As has been shown, the present initial condition of a resonant phonon pulse on a homogeneous chain with nonexcited electronic centers leads to the creation of soliton pairs if the excitation energy is above the threshold. The nonlinear dynamics in this region is now further illustrated in Figs. 4(a)–4(d) for an initial phonon pulse of sech type [see Eq. (4.1)] with fixed $\Delta=8$ and u_0 varying between $u_0=2.31$ and 4.2. From now on we set $\lambda=0.2$ (and $D=4$, $M=1$ as usual) in order to demonstrate the phenomena more clearly. Figure 4(a) shows [like Fig. 1(c) for the $\lambda=0.5$ case] that at threshold and in a small range above the threshold exactly two solitons without any background are created, if the initial phonon pulse has a sech-type envelope. Comparison to Figs. 1(c) and 2 makes evident that the smaller the electron-phonon cou-

pling constant, the broader the solitons, very much like in the SIT case. Other initial phonon pulse shapes (e.g., Gaussian or box-type envelopes) always lead to an additional creation of phonons (linear excitations) besides the soliton pair.

The pair consists of solitons with the same shape of the electronic excitation, the same half-width, but different velocities and different phonon amplitudes, which are proportional to the velocity of the solitons in the rest frame of the system. It is clear that in such a case the phonon amplitude must be larger for faster solitons because the processes of absorption and induced emission must be quicker, which requires larger amplitudes. On the other hand, the slower a soliton the smaller the ratio of vibronic energy to electronic energy. The extreme case is the transition to a localized excited electronic state without any vibronic excitation. This is often the result of decay processes arising from fluctuations during scattering, and will be discussed in the next section.

The existence of very slow solitons with a correspondingly small amount of vibrational energy shows that the nonlinear dynamics of a single soliton is not necessarily connected with a high energy density in the vibrational system, as is assumed in the normal case.

Simulations up to $t=1000$ have shown that these solitons are more stable than in the $\lambda=0.5$ case (see Fig. 2). As solitons are sensitive to interactions with resonant phonons, the reason for the stability may be that contrary to Fig. 2 no background phonons are seen in Fig. 4(a).

If v_f is the velocity of the fast soliton and v_s that of the slower one, we obtain for the case in Fig. 4(a) $v_s=0.40$ and $v_f=1.39$ in units of lattice constants per time unit, where $D=4$ and $M=1$ yield a sound velocity (group velocity around $k_0=\pi/3$) of $c=1.73$.

Increase of the initial phonon amplitude [$u_0=3.15$ in Fig. 4(b)] reduces the half-width of the solitons and increases the velocity *difference* between the solitons of the pair, i.e., the slower soliton nearly comes to rest [$v_s=0.09$ in Fig. 4(b)] while the faster one approaches sound velocity with $v_f=1.62$. Detailed studies of the soliton velocities reveal that $v_s=c-v_f$ holds, similar to the sine-Gordon case. Above threshold [Fig. 4(b)] there appears an additional excitation between the two solitons comparable to the "linear excitation" of Fig. 1(a). A gen-

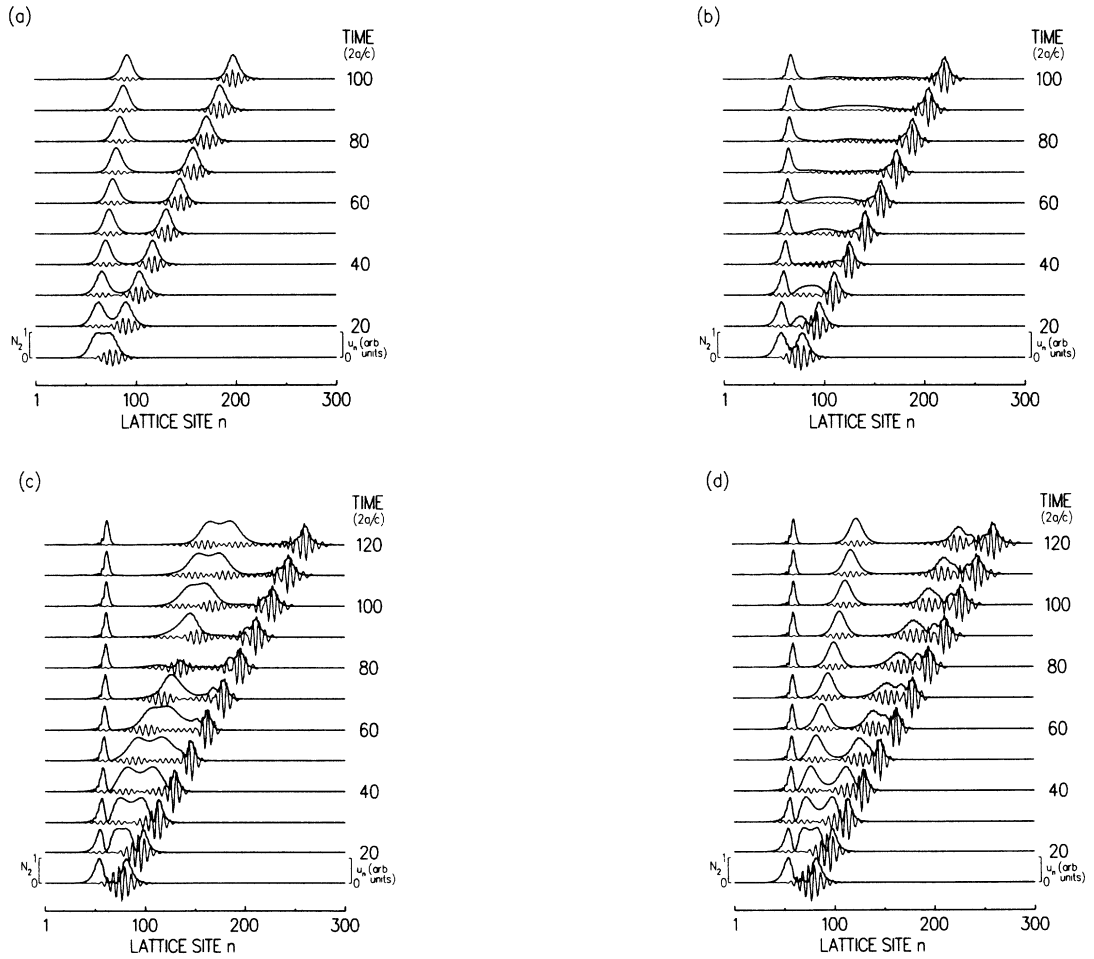

FIG. 4. Same as Fig. 1, but $\lambda=0.2$ and (a) $u_0=2.31$, close above threshold: Two solitons are formed without any background excitations. (b) $u_0=3.15$: two solitons plus additional linear excitations are formed. (c) $u_0=4.03$: an additional breather—instead of linear excitations—is formed. (d) $u_0=4.2$: two pairs of solitons are seen. The two leading excitations interact, lose the proper soliton shape, but are still stable.

eral feature of our above-threshold computer simulations is that such background excitations partially localize around the faster soliton. As a consequence, the faster soliton becomes broader than the small one [see Fig. 4(b)]. This is in agreement with the results of Ruckh and Sigmund,[3] who have analytically shown (with the RWA and continuum approximation) that the phonon dispersion relation is influenced by the soliton in such a way that phonons are localized around the soliton.

Comparison of Figs. 4(b)–4(d) shows a certain repetition of the hierarchy of excitations of Figs. 1(a)–1(c) that appear now between the two solitons of a pair: linear excitation [Fig. 4(b)], a breather [Fig. 4(c)], and a second pair of solitons [Fig. 4(d)]. The difference from the case of Fig. 1 is the partial localization of a part of the linear excitation or the breather around the leading soliton.

This leads to certain deformations of the leading soliton, which is nevertheless as stable against scattering processes and fluctuations as customary solitons, although it is approaching sound velocity, as our numerical studies have shown. The reason could be that the vibrational part of this coupled excitation becomes more dominant the more energy is included from phonons or breathers. As a result, the dynamical equilibrium between the electronic and vibronic parts becomes less important, and the sensitivity against fluctuations decreases correspondingly, especially for very high excitation energies. It may even happen that no complete inversion is obtained anymore.

In the case of *two* pairs of solitons [Fig. 4(d)] the two leading solitons are not clearly separated. Corresponding to the localization of parts of the phonon excitations or breathers around the fast soliton, an attractive interaction occurs between fast solitons with the same direction of motion. Thus the two leading solitons influence one another with the result that they lose the proper soliton shape. Nevertheless it is seen that they form excitations with nearly the same dynamical stability (also during scattering processes) as proper solitons.

Concluding, one can say that fast solitons (i.e., $v \approx c$) attract both one another and subthreshold excitations (phonons and breathers). Therefore, the velocity difference between the two leading solitons is much smaller than the relative velocity of the two slower solitons which separate very well [see Fig. 4(d)].

Further increase of the initial amplitude u_0 results in the creation of a third pair of solitons. The slower ones of the already existing two pairs become even slower and narrower, while the leading excitation as a combination of the fast solitons will further approach c.

VI. SCATTERING PROCESSES

In the following, we take as an initial condition the solitons described in Sec. V, which are then placed at separate initial positions on the lattice ($\lambda = 0.2$). We distinguish between unidirectional and bidirectional scattering processes: The reference system for this distinction is the rest frame of the lattice. In the unidirectional case the solitons taking part in the scattering process have different velocity values, but the *same* direction of motion. In the bidirectional case they have a different or the same velocity value, but *opposite* directions of motion. This cannot be considered by theories that use the RWA because to obtain solutions with different directions of motion it is necessary to solve *second-order* field equations.[8] RWA field equations commonly are of first order. It happens that just the case of bidirectional scattering is interesting because here the solitons lose energy (we call this an inelastic process) and may even decay.

A. Unidirectional scattering

Because of the periodic boundary conditions, Fig. 5 can simply be obtained by continuation of the simulation shown in Fig. 4(a). After the collision the original shapes of the solitons are perfectly recovered without any energy loss, i.e., this scattering process is elastic. The interaction between the solitons produces phase shifts: The center of the fast soliton is shifted in the direction of motion (i.e., to the right in Fig. 5), whereas the slower one is moved opposite the direction of motion (i.e., to the left in Fig. 5). It is interesting that during the scattering process there is a moment where the whole excitation energy has been transferred to the vibrational system. It is then the same state as at the beginning ($t = 0$) of the simulation in Fig. 4(a). The results are very similar to those obtained by conventional analytic approaches in the field of SIT where the model system is reduced to a sine-Gordon system. Moreover, it is shown here that elastic scattering is maintained even for ultrashort solitons.

B. Bidirectional scattering

As an example of bidirectional scattering between fast solitons [Fig. 6(a)], we chose solitons like the fast one in Fig. 4(a) moving in different directions. There is no special reason for choosing the same velocity value. Different, but sufficiently large velocity values lead to the same qualitative behavior.

During the scattering process, a highly oscillatory elec-

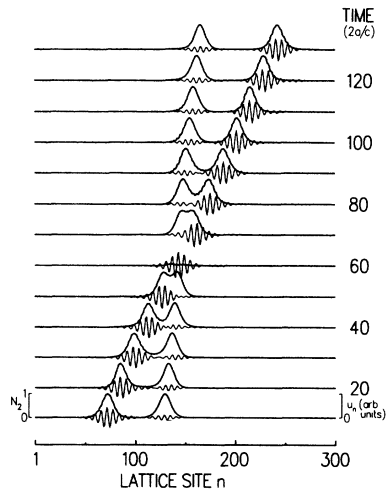

FIG. 5. Unidirectional scattering process between the slow and fast solitons of Fig. 4(a). Except for a phase shift, the solitons are left unaffected.

tronic excitation is created where the minima are approximately at those points where the displacement u_n passes zero. This is because during the scattering process the electronic excitation is coupled to a standing vibrational mode. Simulations with a standing phonon mode as an initial condition lead to the same oscillatory pattern of the electronic excitation as is seen in the center of the scattering complex. Finally, a part of the electronic excitation decouples from the solitons and marks the place of the soliton-soliton collision. There is nearly no induced emission of the localized, split-off electronic excitation because of the lack of phonons—the latter remain part of the soliton dynamics. However, these electronic excitations would decay by spontaneous processes which are neglected in this approach. What remains is that a part [about 6% in Fig. 6(a)] of the total soliton energy is split off: bidirectional scattering processes are, in this sense, slightly inelastic. This also holds for SIT bidirectional scattering.[8]

In the case of bidirectional scattering, phase shifts are seen too: The center of each soliton is shifted in the direction of motion.

Because of the energy loss of the solitons the question arises whether a slow soliton may decay into linear excitations during a bidirectional soliton-soliton scattering process. Figure 6(b) shows that this is indeed the case. The solitons are the same as in Fig. 5, but with different directions of motion. The weak phonon part of the slow soliton is not able to restore the original soliton shape from the highly oscillatory electronic intermediate state. Obviously the colliding solitons, whatever their velocity, together lose about the same absolute amount of energy ΔE, which is roughly determined by the spatial extension Δx of the highly oscillatory electronic state in the scattering region: $\Delta E \lesssim \hbar\Omega\,\Delta x$. This means that the slow soliton loses so much energy to the electronic excitation which remains at the location of the scattering process that the phonon part of the decaying soliton is not able to restore dynamical stability. In other words, in the case of slow solitons the localization of the phonon part by the electronic excitation is stronger than in fast solitons. If the electronic excitation is disturbed (e.g., by a bidirectional scattering process with solitons or phonons), it is more difficult to keep the balance between absorption and induced emission for slow solitons than it is for fast ones. The result may be the decoupling of the electronic from the vibronic excitation, i.e., the decay of the slow soliton.

The striking stability of the localized states that are left over by the scattering process is interesting. Although the vibronic excitation clearly could induce emission by the electronic centers, this does not happen: The localization effect of the electronic centers on the phonons is obviously more important in this case.

Figure 7 illustrates a soliton–resonant-phonon scattering process. Again there is a small soliton phase shift in

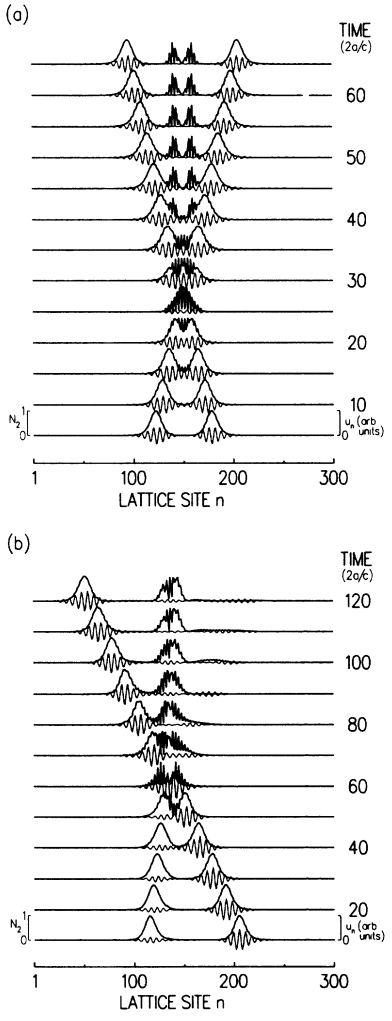

FIG. 6. (a) Bidirectional scattering process between two fast solitons of Fig. 4(a) as an initial condition. Note the trapped electronic excitation which marks the collision region: inelastic scattering. (b) Bidirectional scattering process between the slow and fast solitons of Fig. 4(a). The slow soliton decays because of the energy loss.

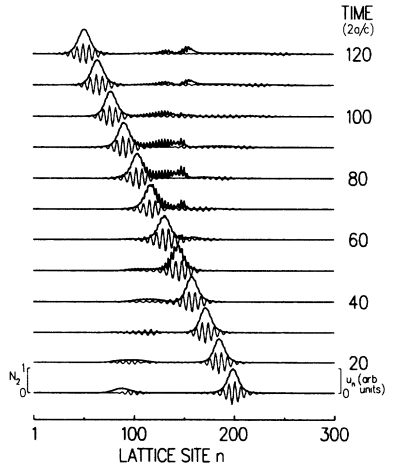

FIG. 7. Bidirectional soliton-phonon interaction: the initial condition is the fast soliton of Fig. 4(a); the phonon excitation starts with $u_0 = 0.63$. Note the strong electronic fluctuations between $t = 70$ and $t = 90$.

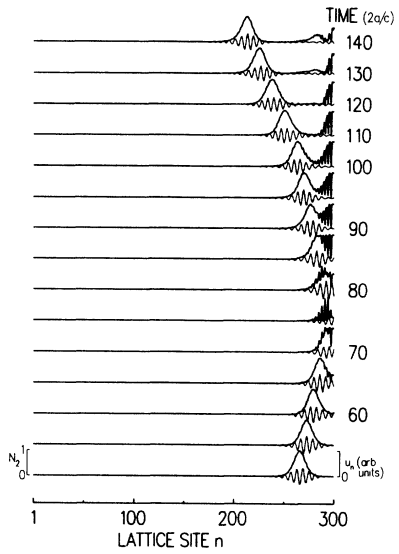

FIG. 8. Inelastic reflection process from the free surface of a finite lattice: the initial condition is the fast soliton of Fig. 4(a). Note the highly oscillatory electronic excitation at $t=75$, which is partly transformed back to soliton shape later on.

the direction of motion. The energy loss of the soliton is very small; more important are the relatively large fluctuations, here for $t=70$ up to $t=90$. In Sec. IV [Fig. 1(c)] we have already seen that this kind of fluctuation may lead to the decay of solitons, especially in the case of narrow solitons and a larger concentration of phonons. Solitons with a larger half-width (i.e., smaller λ) are not so sensitive to interactions with phonons. To conclude, the energy loss of solitons when scattered by phonons is not so important as the fluctuations that are introduced into the dynamics of the soliton. In general, the scattering from resonant phonons (linear excitations) is much more important for the decay of solitons than the influence of the discreteness of the electronic center distribution.

VII. REFLECTION PROCESSES

In this section the behavior of solitons in finite systems with free-surface boundary conditions is investigated. The result is a kind of "soliton echo" (cf. Fig. 8).

Due to symmetry arguments, reflection processes from the "open end" of a pure vibronic system are analogous to bidirectional scattering processes of identical phonon pulses (if certain phase conditions are fulfilled). This analogy no longer holds for coupled coherent excitations. During the scattering process the electronic excitations of the two solitons interact via the vibrational system, and in the case of reflection *only* the electronic excitation of the one soliton is interacting with both the incoming and reflected vibrational excitations. This means that during the reflection process we are dealing with a standing vibrational mode. The result is again a highly oscillatory electronic excitation which, however, is transformed back to a perfect soliton shape by the reflected phonon pulse, except for a trapped rest excitation which finally decays into phonons. The conclusion is that, besides some energy loss, these reflection processes retain the soliton properties.

VIII. CONCLUSIONS

This numerical investigation shows the existence of ultrashort solitons. These are coupled coherent propagating excitations in both the electronic and the phonon systems that interact by absorption and induced emission processes forming a dynamically metastable state. Stability is preserved for half-widths down to one wavelength of the carrier phonons, which are in resonance with the energy splitting of the electronic systems.

Very similar to the SIT case, there exists also for ultrashort excitations a threshold behavior and a hierarchy of excitations with qualitatively different behavior: linear excitations, which blur over the whole system; breathers, that periodically change their shape; and above the threshold solitons.

Increasing the electron-phonon coupling constant results in a decreasing half-width of the soliton solutions connected with an increasing instability of the solitons against fluctuations induced by phonons (linear excitations).

Incident phonon pulses pass interfaces (where λ changes from zero to a finite value) without reflection. Their amplitude defines the resulting soliton energy. If the pulse width lies within a soliton window, the phonon pulse is converted into a soliton without any background excitation.

Scattering experiments reveal elastic unidirectional and inelastic bidirectional processes. In the case of slow solitons with a small phonon amplitude, bidirectional scattering may even lead to the decay of the solitons into localized electronic excitations and decoupled phonons.

Investigations of finite systems have shown that in the case of soliton reflection from the free surface of the lattice the process is inelastic, i.e., besides the reflected soliton, linear excitations are formed.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft in Sonderforschungsbereich 329, "Physikalische und chemische Grundlagen der Molekularelektronik."

[1]L. Kahn, N. S. Almeida, and D. L. Mills, Phys. Rev. B **37**, 8072 (1988).

[2]S. L. McCall and E. L. Hahn, Phys. Rev. **183**, 457 (1969).

[3]R. Ruckh and E. Sigmund, Phys. Rev. B **35**, 4380 (1987).

[4]M. Engelhardt, U. Happek, and K. F. Renk, Phys. Rev. Lett. **50**, 116 (1983).

[5]G. L. Lamb, Jr. and D. W. McLaughlin, in *Aspects of Soliton Physics* Vol. 17 of *Topics in Current Physics*, edited by R. K.

Bullough and P. J. Caudrey (Springer, Berlin, 1980), pp. 65–106.

[6]A. Kujawski, Z. Phys. B **66**, 271 (1987).

[7]K. Steiglitz, I. Kamal, and A. Watson, IEEE Trans. Comput. **TC-37**, 138 (1988).

[8]R. K. Bullough, P. M. Jack, P. W. Kitchenside, and R. Saunders, Phys. Scr. **20**, 364 (1979).

[9]For simplicity, in Eq. (2.1) the number of electronic centers equals the number of lattice points, while in real physical applications the center concentration may be much smaller. However, the addition of equal numbers of lattice points between neighboring electronic centers will not change the basic results, except for a rescaling of parameters. This is because lattice dispersion is not important for the nonlinear dynamics discussed in this paper.

[10]H. Haken and A. Schenzle, Z. Phys. **258**, 231 (1973).

[11]G. Engeln-Müllges and F. Reutter, *Formelsammlung zur Numerischen Mathematik*, 4th ed. (Bibliographisches Institut, Mannheim, 1984), p. 248.

[12]"ch" stands for change.

[13]N. Theodorakopoulos and R. Klein, Phys. Status Solidi A **61**, 107 (1980).