Physics Letters A 181 (1993) 232-238
North-Holland

PHYSICS LETTERS A

Localized excitations in a discrete Klein-Gordon system

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Received 4 May 1993; accepted for publication 6 August 1993
Communicated by A.R. Bishop

We analyze the origin and features of localized excitations in a discrete Klein-Gordon system. We connect the presence of these excitations with the existence of local integrability of the original N-degree of freedom system. On the basis of this explanation we make several predictions about the existence and stability of these excitations.

1. Introduction

Solitary waves and solitons play a significant role in various physical problems [1,2]. Nonlinear forces acting on fields (continuum problem) or interacting particles (discrete problem) are necessary for the existence of solitons. A large variety of nonlinear continuum models exhibits soliton-like features. For example practically all Klein-Gordon systems with multiwell on-site potentials exhibit single kink solutions. However only for special potentials (like sine-Gordon) do these kinks become real solitons, i.e. the corresponding system becomes integrable. Besides kinks in the sine-Gordon system (sG) so-called breathers are found to be exact solutions. These breathers can be viewed as bound states of a kink and an antikink. The important difference between kinks and breathers is, that breathers are local excitations above the ground state having the same symmetry as the ground state. Kinks (and antikinks) are "links" between different equal ground states, so that these local excitations do not have the same symmetry as any ground state. Kinks are therefore important concerning second order phase transitions, where symmetry breaking takes place. However, dynamical properties of the above mentioned systems may be affected by the presence of both kinks and breathers.

A large number of physical applications have models that correspond to discrete nonlinear systems. In that case the translational symmetry is broken, and thus the mathematical properties of nonlinear localized excitations (NLE) like kinks or breathers have to be reconsidered with respect to discreteness. That has been a topic for a huge number of scientific publications. Recently a new class of self-localized modes in discrete nonlinear lattices has been introduced and studied by Takeno and coworkers (see refs. [3,4], and references therein). The eigenfrequency of those modes usually was found to be above the upper phonon band edge frequency. In that case the found modes have no counterparts in the corresponding continuum models. The shapes and frequency of these modes were calculated using the rotating wave approximation (RWA) [5].

We want to present a careful analysis of nonlinear localized excitations for a discrete one-dimensional system. The frequency of the NLEs can be either below or above the optical phonon band frequencies. We will show that the existence of those excitations is due to the integrability of the original N-degree of freedom system in parts of the phase space (local integrability). The existence of KAM-tori is shown using Fourier analysis and Poincaré intersections. We propose a perturbation-like scheme, which can be adopted for very discrete systems as an easy way to account for the main features of the NLE. We formulate stability conditions of the NLE, which mainly use the integrability character of the solutions and their coupling to small amplitude phonons. An im-

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portant finding is an energy threshold for the existence of the NLE. This threshold depends on the degree of discreteness and can be qualitatively explained within the above mentioned perturbation-like scheme.

2. Model and localized solutions.

We study a $d=1$ dimensional discrete classical model given by the Hamiltonian

$$H=\sum_{l=1}^{N}\left[\tfrac{1}{2}P_l^2+\tfrac{1}{2}C(Q_l-Q_{l-1})^2+V(Q_l)\right]. \tag{2.1}$$

P_l and Q_l are canonically conjugated momentum and displacement of the lth particle, where l marks the number of the unit cell. C measures the interaction to the nearest neighbour particles. All variables are dimensionless. The mass of the particles is equal to unity. N is the total number of particles. The nonlinearity is hidden in the "on-site" potential $V(x)$. Here we choose the Φ^4 type potential,

$$V(x)=V_{\Phi^4}(x)=\tfrac{1}{4}(x^2-1)^2. \tag{2.2}$$

For convenience we restrict ourselves to potential (2.2). It will be seen from the analysis that in principle the methods can be applied to other systems with analogous results. Especially NLE were found for Fermi–Pasta–Ulam systems (where the nonlinear local potential $V(x)$ is replaced by nonlinear springs) [6] and for hard quartic anharmonicity $V(x)=x^4$ [3]. Higher dimensionality $d\geqslant 2$ should also be no principal hurdle [4].

Nonlinear localized excitations can be very easy produced (if the system allows for their existence) by numerically choosing an initial condition which corresponds to a localization of energy. Here we simply positioned the whole system into its ground state and then displaced one (central) particle by a given amount of displacement. Then the evolution of the system can be studied by means of molecular dynamics. We used always periodic boundary conditions. Since some amount of the initial energy will be transformed into travelling phonons (radiation), one has to take care of the system size to exclude effects of return. We have done it by choosing a large enough system. We used the Verlet algorithm [7] for solving the Newtonian equations of motion. The time step was $h=0.005$. The system size was $N=3000$.

Before coming to examples of NLE, let us mention the properties of (2.1) for small amplitude oscillations around the ground state. A simple calculation yields the following dispersion law for small amplitude phonons,

$$\omega_q^2=\omega_0^2+4C\sin^2(\pi q/N), \tag{2.3}$$

where $q=0, 1, 2, ..., N-1$ is the wave number, ω_q is the frequency of a phonon with wave vector q and ω_0 measures the lower phonon band edge: $\omega_0=\sqrt{2}$. As (2.3) indicates, one major difference between the considered discrete system (2.1) and its continuum counterpart ($C\to\infty$) is the existence of a finite upper phonon band edge. This fact is responsible for the possibility of exciting NLE with frequencies above the phonon band in contrast to the continuum case. However here we will study NLE with frequencies in the gap. We will see that although the continuum counterparts do exhibit a gap, the nature of the NLE in the discrete system is not trivially connected with possible NLE in the continuum system.

Now let us show a typical example of NLE for a special choice of the interaction strength $C=0.1$. This value was considered because it corresponds to a balance between the on-site energy of a particle and the energy of the springs connecting it to the neighbours for energies of the order of the barrier height of $V(x)$. To characterize the behaviour of the system we introduce a local energy variable e_l,

$$e_l=\tfrac{1}{2}P_l^2+V(Q_l)+\tfrac{1}{4}C[(Q_l-Q_{l-1})^2+(Q_l-Q_{l+1})^2]. \tag{2.4}$$

Obviously the sum over all local energies gives the total conserved energy. If NLEs are excited, the initial local energy burst should mainly stay within the NLE. Thus defining

$$e_{(2m+1)}=\sum_{-m}^{m}e_l \tag{2.5}$$

and exciting the local energy burst at lattice site $l=0$ by choosing a proper value of m in (2.5) we will control the time dependence of $e_{(2m+1)}$. Here $2m+1$ determines the size of the NLE. If this function does not decay to zero (or decays slowly enough), the existence of a NLE can be confirmed. The expression "slowly enough" has to be specified with respect to

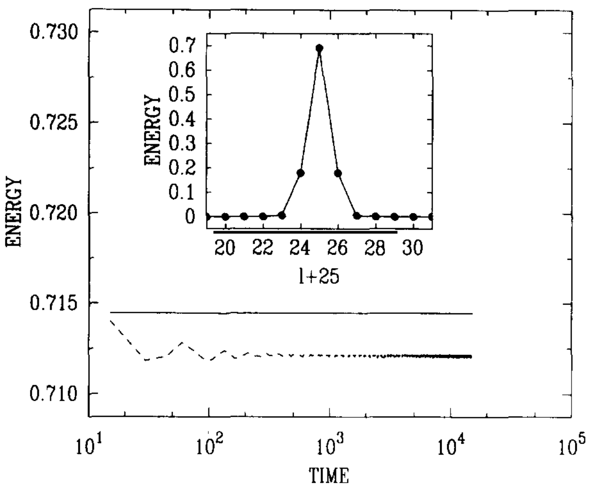

Fig. 1. $e_{(5)}$ versus $\log_{10}(t)$ for $Q_0(t=0)=1.3456$ (dashed line). Total energy of the system (solid line). Inset: Maximum values (full circles) of e_l for $t \geqslant 1000$ with initial condition as in fig. 1. Solid line is a guide to the eye.

the typical group velocities of small amplitude phonons. This sets the time scale we are interested in,

$$t \gg m \frac{\sqrt{\omega_0^2+2C}}{2C} . \tag{2.6}$$

In fig. 1 we show the time dependence of $e_{(5)}$ for $Q_{l\neq 0}(t=0)=-1$, $Q_{l=0}(t=0)=1.3456$, $\dot{Q}_l(t=0)=0$. This choice of initial condition corresponds to a motion of the central particle over both wells of potential (2.2). Clearly a NLE can be detected. After a short time period of the order of 100 nearly constant values of $e_{(5)}$ are observed. The NLE seems to be extremely stable. To characterize the energy distribution within the NLE we plot the maximum values $e_l^{\max}$ of the local energies e_l in the inset in fig. 1. Essentially three particles are involved in the motion. We are confronted with a rather localized excitation.

3. Stability analysis

NLE solutions in different systems were studied using rotating wave approximation (RWA) [3]. We leave a critical discussion of the applicability of RWA for a future paper, and concentrate in this section on one basic assumption within the RWA concept. Namely, that the NLE solution can be represented by a coherent motion of all involved particles. This motion is characterized by one fundamental frequency $\omega_1=2\pi/T_1$ (see, e.g., ref. [4]),

$$Q_l(t)=Q_l(t+T_1) . \tag{3.1}$$

Let us analyze the stability of such a solution with respect to small amplitude phonons, which can be viewed as a characterization of external (with respect to the NLE) parametric resonances.

Let us assume that we found an exact NLE solution $Q_l(t)$ with property (3.1). To study the stability of such a solution with respect to small amplitude oscillations (phonons) we consider a small deviation from this solution $Q_l(t)+\Delta_l(t)$, insert this ansatz in the original equations of motion and linearize with respect to Δ. Finally we transform the equations into q-space and find

$$\ddot{\Delta}_q+\omega_q^2\Delta_q+\sum_{q'}\Delta_{q'}\left(\frac{2\alpha_1}{N}Q_{q-q'} + \frac{3\alpha_2}{N^2}\sum_{q''}Q_{q''}Q_{q-q'-q''}+\ldots\right)=0 , \tag{3.2}$$

where the constants α_i are defined through the derivatives of the potential at the ground state position. We introduce a vector

$$\Delta=(\Delta_{q_1},\dot{\Delta}_{q_1},\ldots,\Delta_{q_N},\dot{\Delta}_{q_N}) \tag{3.3}$$

Then we can rewrite (3.2) as

$$\dot{\Delta}=\mathbf{M}(\{Q_q(t)\})\Delta . \tag{3.4}$$

The matrix $\mathbf{M}$ has several interesting properties. The trace of the matrix is zero. The matrix is also periodic in time with period $T_1=2\pi/\omega_1$. Let us introduce a mapping A

$$A\Delta(t)=\Delta(t+T_1) . \tag{3.5}$$

Following Arnol'd [8], a solution $\Delta(t)$ is stable (with period T_1) if the mapping A is stable. Since the matrix $\mathbf{M}$ is linear, the mapping A is volume preserving and the necessary condition of stability of a solution of (3.4) becomes

$$|\mathrm{tr}\,A|<2N . \tag{3.6}$$

Since $Q_l(t)$ is a localized solution, its transformed counterpart $Q_q(t)$ is finite for every q, whereas a wave solution would be N times larger. Thus the $1/N$, $1/N^2$, ... terms in (3.2) let the additive perturbation terms in the differential equations of (3.2) and (3.4) become very small for large enough N. Then, it is possible to study the stability of the mapping A neglecting the perturbation. Since the mapping matrix in that case becomes block-diagonal, the sufficient condition of stability of a solution of (3.4) reduces to

$$\frac{\omega_q}{\omega_1} \neq \frac{n}{2}, \quad n=0, 1, 2, \ldots . \tag{3.7}$$

This stability condition implies the existence of instability bands on the frequency axis of the NLE because of the finite dispersion. It tells nothing about lifetimes of strictly speaking unstable NLE. Nevertheless it can be used as a test whether the found NLE stability can be explained by condition (3.7).

4. The integrability concept

To characterize our NLE solution found numerically we perform a Fourier analysis of the motion of the central particle $l=0$ and the nearest neighbours $l=\pm 1$. Because of the symmetry of the initial condition the two nearest neighbours move in phase. In fig. 2 the Fourier transformed (FT) trajectories of the central particle and of the nearest neighbours (inset in fig. 2), respectively, are shown. The peak

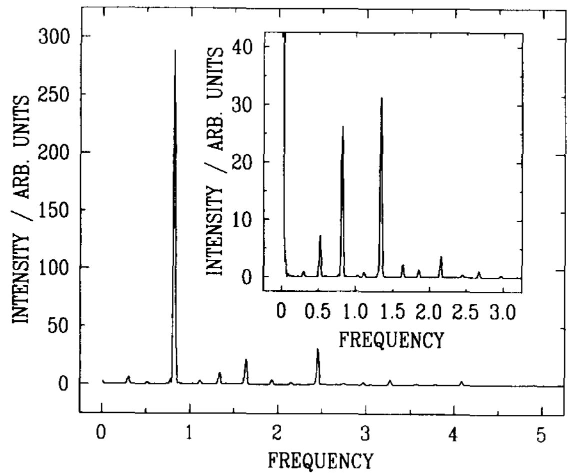

Fig. 2. Fourier transformed $\mathrm{FT}[Q_l(t\geqslant 1000)](\omega)$ with initial condition as in fig. 1 for $l=0$. Inset: for $l=\pm 1$ (same intensity units as in fig. 2).

positions cannot be explained by multiples of one fundamental frequency ω_1, as suggested by the RWA ansatz (3.1). However, all peak positions can be explained as a linear combination of multiples of two frequencies – $\omega_1=0.822$ and $\omega_2=1.34$. Although it is impossible to extend the stability analysis of the previous section to an (assumed) localized solution with two fundamental frequencies, we note that no one of the visible peaks in fig. 2 overlaps with the instability bands defined by (3.7).

To understand the appearance of the second frequency we recall that the NLE is a three particle excitation (cf. inset in fig. 1), and because of the symmetry of the initial condition we are left with a two degree of freedom problem. Now it is a small step to recognize, that we might be confronted with a kind of integrability phenomenon. Indeed, fixing the rest of the particles at their ground state positions reduces the dynamical problem to a two degree of freedom system (reduced problem), which might be integrable in parts of its phase space,

$$\ddot{Q}_0 = -V'_{\Phi^4}(Q_0) - 2C(Q_0 - Q_{\pm 1}) , \tag{4.1}$$

$$\ddot{Q}_{\pm 1} = -V'_{\Phi^4}(Q_{\pm 1}) - C(Q_{\pm 1} - Q_0 + 1) . \tag{4.2}$$

To show that this is indeed true, we solve numerically the Newtonian equations of motion of this reduced problem and perform a Poincaré intersection between the trajectory and the subspace $\{\dot{Q}_0, Q_0, Q_{\pm 1}=-1, \dot{Q}_{\pm 1}>0\}$. The result is shown in fig. 3a. Clearly we find the existence of integrable motion on a torus. To be sure that we are on the right track, we perform the same procedure for the 3000-degree of freedom system with same initial conditions. The torus intersection in fig. 3b is nearly indistinguishable from the two degree of freedom result in fig. 3a. Thus we arrive at two conclusions: (i) the NLE existence is a result of (at least local) integrability properties of the underlying many-particle system; (ii) the NLE can be reproduced within a reduced problem, where all particles performing small amplitude oscillations are fixed at their ground state positions, thereby reducing the number of relevant degrees of freedom.

With the integrability property in mind, it is clear that there have to appear two frequencies. If the reduced problem is integrable (in some part of phase space) there should appear two actions I_n, $n=1, 2$, as functions of the original variables, so that the

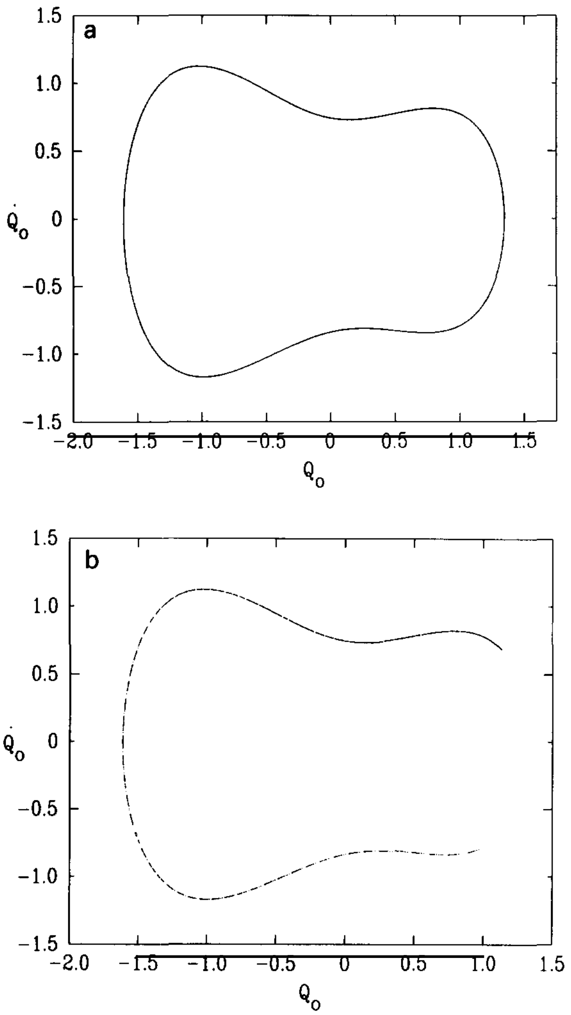

Fig. 3. Poincaré intersection between the trajectory and the subspace $\{\dot{Q}_0, Q_0, Q_{\pm1}=-1, \dot{Q}_{\pm1}>0\}$ with same initial condition as in fig. 1. (a) Reduced three particle problem (see text); (b) full problem ($N=3000$).

Hamiltonian of the reduced problem can be expressed through the two action variables only, and these actions become integrals of motion (see, e.g., ref. [9]). The corresponding two frequencies

$$\omega_n = \frac{\partial H}{\partial I_n} \tag{4.3}$$

determine the motion of system on the surface of the torus. Obviously all linear combinations of multiples of these frequencies appear in the Fourier spectrum of the original particle displacements. That is exactly what we observe. Before turning to approximate descriptions of the motion under study, let us mention that the conclusions from above imply another consequence – namely, that an asymmetric NLE (with respect to the central particle) should be possible too, i.e. that the two nearest neighbours perform out of phase motions, even with different amplitudes. That would mean, that in the language of actions we lift a degeneracy by choosing asymmetric initial conditions and have to expect three instead of two fundamental frequencies, i.e. the frequency ω_2 splits into two frequencies $\omega_2 \neq \omega_3$. To check this statement we performed a simulation with an asymmetric initial condition, which differs from the previous symmetric initial condition by additionally choosing $Q_1(t=0) = -0.7 \neq -1$. Indeed we find (i) that the local asymmetry is conserved throughout the evolution of the system, and as the Fourier spectrum of the central particle motion and the two nearest neighbours motions shows, we now find three frequencies: $\omega_1 = 0.83$, $\omega_2 = 1.32$ and $\omega_3 = 1.35$.

Next we want to discuss approximation schemes to account for the basic features of the above NLE. Since we are dealing with a NLE such that $\delta Q_0 \gg \delta Q_{\pm1}$ where $Q_l = -1 + \delta Q_l$, a starting point could be to consider the equation of motion for the central particle neglecting the small amplitude fluctuations of the nearest neighbours. We arrive at the effective one particle problem

$$\ddot{Q}_0 = -\frac{\mathrm{d}V_{\mathrm{eff}}}{\mathrm{d}Q_0}, \tag{4.4}$$

where the effective potential V_{eff} is given by the expression

$$V_{\mathrm{eff}}(x) = V(x) + C(x+1)^2 . \tag{4.5}$$

Using the amplitude of the central particle as an input parameter, one can solve eqs. (4.4), (4.5) with respect to the fundamental frequency ω_1. To account for the second frequency let us consider the equation of motion for the nearest neighbour using $\delta Q_1 \gg \delta Q_2$,

$$\delta\ddot{Q}_1 = -\frac{\mathrm{d}V}{\mathrm{d}Q_1}\bigg|_{Q_1=\eta+\delta Q_1} - 2C\delta Q_1 + CQ_0 . \tag{4.6}$$

This equation describes a driven nonlinear oscillator, where CQ_0 is the driving term. If the amplitude of the nearest neighbour is small enough, the nonlinearity coming from $V(Q_1)$ can be approximately handled by replacing the original anharmonic potential by a harmonic one with amplitude-dependent frequency. Nevertheless, we are still confronted with a complicated problem, since the driving term is not a harmonic function. Thus if we assume that the driving term in (4.6) is a harmonic function with frequency ω_1, we can solve the equation of motion for Q_1. Using the full amplitude of the nearest neighbour as an input parameter, one can solve for the second frequency ω_2.

To check our scheme, we use the simulation result for Φ^4 and $Q_0(t=0)=1.3456$. The simulation yields $\omega_1=0.822$, $\omega_2=1.34$. The approximation scheme gives $\omega_1=0.82$, $\omega_2=1.31$. These results should not be overestimated – in our opinion they only show, that the integrability concept is correct, and the existence of more than one fundamental frequency characterizing the NLE is natural.

The above described approximation scheme can also successfully be used to account qualitatively for stability properties of the NLE. For that we plot in fig. 4 the energy dependence of the fundamental frequency of the effective potential (4.5). We observe, that for energies smaller than some threshold value the frequency lies always in the phonon band. The same effect appears for an energy window at larger energy values. Using the stability condition (3.7) we

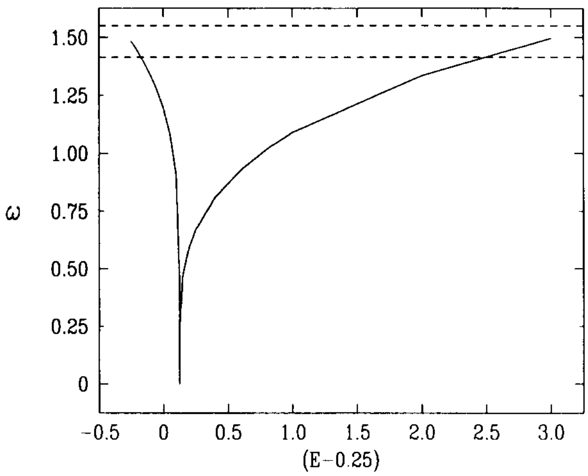

Fig. 4. Energy dependence of the fundamental frequency ω_1 for the effective potential (4.5) (solid line); dashed lines indicate the position of the phonon band (2.3).

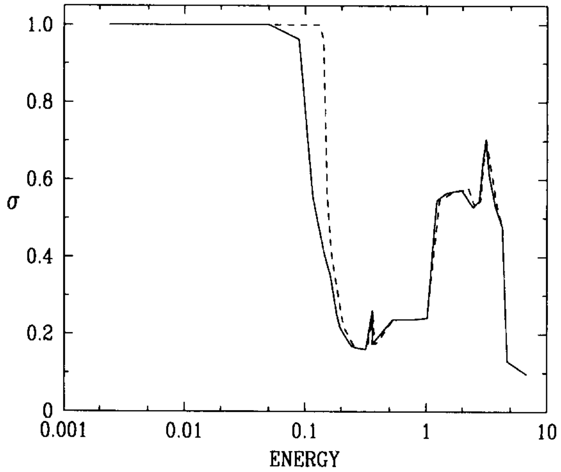

Fig. 5. Energy dependence of the normalized entropy σ. For the solid line the abscissa is the NLE energy scale; for the dashed line the abscissa is the initial energy scale.

conclude that there exists an energy threshold for the creation of a NLE, as well as a second instability window at larger energies, or in other words, the excitation spectrum of the NLE has two gaps. To check this conclusion, we calculate the normalized local energy distribution functions $p_l = e_l^{\max}/\sum_l e_l^{\max}$ for different initial energies e. Then we calculate the corresponding normalized entropy σ of these distributions

$$\sigma = -\frac{1}{\ln(N)} \sum_l p_l \ln(p_l) . \tag{4.7}$$

From definition (4.7) we have $0<\sigma<1$. Delocalization occurs if $\sigma=1$ and maximum localization if $\sigma=0$. Then we plot in fig. 5 the energy dependence of σ. The solid curve in fig. 5 represents the dependence of σ on the energy of the NLE, whereas the dashed curve shows the dependence of σ on the initial energy. We clearly observe the two gaps in the excitation spectrum of the NLE. The difference between both curves indicates the amount of energy lost by initial radiation.

5. Discussion

The integrability concept sketched above is not restricted to the Φ^4 model. It is also not restricted to the dimensionality of the system. It provides a simple understanding of the phenomenon of localization in terms of regular motion. The main reason for the occurrence of NLEs is the nonlinearity of the system, which expresses itself by an energy dependence of oscillation frequencies of the particles. In that sense the existence of a NLE can be viewed as a consequence of (nearly) zero energy transfer between coupled oscillators with different frequencies. Here we find a common feature with well-known localized excitations in harmonic systems with mass defects (see, e.g., ref. [10]). The energy dependence of the frequencies in nonlinear systems can be partially matched to an energy dependence of particle masses. Thus when we choose an initial condition with strongly varying energies we end up with a solution close to a corresponding harmonic system with mass defect.

The success of the approximation scheme encourages us to proceed to the prediction of the existence of NLEs in other systems. For example, that (2.1) with

$$V(Q_l) \Rightarrow V(Q_l - Q_{l-1}) = (Q_l - Q_{l-1})^k \qquad (5.1)$$

allows for no NLE solutions for $k=3$, but allows for solutions for $k=4$. That happens because the fundamental frequency of the corresponding effective potential for the central particle will never come out of the phonon band for $k=3$. In contrast the frequency comes out of the phonon band for $k=4$ for large enough initial amplitudes. Such predictions will be checked in forthcoming work.

When we compare the value of the energy threshold for NLE creation with the minimum energy of a kink–antikink pair $E_{\mathrm{K\bar{K}}}^{\min}$, we find that for the parameter case studied here $E_{\mathrm{K\bar{K}}}^{\min}$ is nearly four times larger than the value of the energy threshold of the NLE. Thus one can expect that at certain temperatures the NLE can affect the dynamical behaviour of the system stronger than do kinks and antikinks.

One critical comment should be added with respect to the stability analysis in section 3. From (3.7) it follows, that there are no stable NLEs in the continuum limit $C \to \infty$ with frequencies below the lower phonon band edge frequency. However it is well known, that some models like the sine-Gordon model allow for exact breather solutions in the continuum limit [11]. The reason for that should be the vanishing of the prefactors of the resonant terms in the perturbation expansion for such nongeneric integrable continuum models.

Finally we want to emphasize, that we have found rather interesting objects from the point of view of nonlinear motion. The NLEs appear to behave like three particle excitations weakly coupled to phonons. Because of the weak coupling we expect to find adiabatic tuning of the energy of the NLE as well as of its actions and frequencies. Together with the existence of several internal degrees of freedom this can be an interesting object for unusual energy relaxation in complex systems.

Acknowledgement

This work was supported in part (S.F.) by the Deutsche Forschungsgemeinschaft (Fl 200/1-1).

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