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Conditions on the existence of localized excitations in nonlinear discrete systems

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We use recent results that localized excitations in nonlinear Hamiltonian lattices can be viewed and described as multiple-frequency excitations. Their dynamics in phase space takes place on tori of corresponding dimension. For a one-dimensional Hamiltonian lattice with nearest neighbor interaction we transform the problem of solving the coupled differential equations of motion into a certain mapping $M_{l+1} = F(M_l, M_{l-1})$, where M_l for every l (lattice site) is a function defined on an infinite discrete space of the same dimension as the torus. We consider this mapping in the "tails" of the localized excitation, i.e., for $l \to \pm\infty$. For a generic Hamiltonian lattice the thus-linearized mapping is analyzed. We find conditions of existence of periodic (one-frequency) localized excitations as well as of multiple-frequency excitations. The symmetries of the solutions are obtained. As a result we find that the existence of localized excitations can be a generic property of nonlinear Hamiltonian lattices in contrast to nonlinear Hamiltonian fields.

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I. INTRODUCTION

Localization phenomena are of interest in nearly any branch of physics. In this paper we will deal with translationally invariant systems. In that spirit we deal with localization phenomena which appear due to *intrinsic* properties of the underlying system instead of due to *extrinsic* sources (e.g., defects). There has been considerable success in the demonstration of the occurrence of localized vibrations in Hamiltonian lattices [1–6]. The pure fact of the possibility of vibrational localization is astonishing because of the translational invariancy of the underlying lattice (i.e., no defects of any kind are necessary). The necessary localization condition has to be the nonlinearity of the lattice, since in the case of a linear lattice the problem is integrable and only extended degrees of freedom can be found.

Most of the knowledge about vibrational localization is restricted to simple one-dimensional lattices, usually with one degree of freedom per unit cell and nearest neighbor interaction. These systems belong to the class of Fermi-Pasta-Ulam (FPU) models (see, e.g., [7]). If one adds an external potential (field) which is periodic with the periodicity of the FPU system, one enters the world of Klein-Gordon lattices. The important property of vibrational localization in all these systems is that it is not of topological origin, i.e., we can consider a system with only one minimum in the potential energy function (the ground state) and will find vibrational localization. If the potential energy function has several minima one can construct static kink solutions, i.e., static configurations of the system which link different ground states (minima) of the model. Those static kink solutions can be either minima or saddle points in the potential energy function. The concept of vibrational localization is then extendable to those minima (kinks). One simply considers excitations of the lattice above this (kink) minimum. Because the static kink itself breaks the translational invariance of the underlying lattice, a linearization and diagonalization of the fluctuations around kinks usually yields several eigenmodes which correspond to localized vibrations [8–11]. The rest of the eigenmodes are deformed phononlike extended degrees of freedom. Here we find a difference with the nontopological vibrational localization — namely, localization in the linear limit. Of course it only becomes possible because the static kink already broke the translational symmetry. It is worthwhile to notice that the topological-induced vibrational localization is comparable to the well-known vibrational localization in a linear lattice with defects [12].

Recently we were able to achieve progress in the understanding of non-topological vibrational localization [13, 14]. First we noticed that it is possible to find nonlinear localized excitations (NLEs) which are essentially located on a very few particles. By analyzing the dynamics of the lattice *on finite time scales* we found that in general the NLE is a many-frequency excitation, where the number of frequencies n is equal to the number of particles which are essentially involved in the excitation. By studying a reduced system which is given by the dynamics of the part of the lattice where the NLE is located (with properly defined boundary conditions) we showed that the NLEs in the original lattice correspond to regular motions of the reduced system on n-dimensional tori in its phase space. Moreover, the NLE solution of the original lattice evolves on nearly the same torus. Thus it becomes possible to systematically study the NLE properties by checking the phase space structure of the reduced system. As a result we found that chaotic motion in the reduced system does not yield NLEs, as well as certain regular islands in its phase space which are well separated (by separatrices) from the NLE-regular islands. We were

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also able to attack the problem of movability of NLEs by considering a certain separatrix in the phase space [15]. Still the question remains whether NLEs can be *exact* solutions of the lattice equations of motion.

Much less is known about more complicated models. First we notice that the above cited approach in the simplest one-dimensional systems is easily extended to higher dimensions or to more than one degree of freedom per unit cell. Indeed recent reports confirm the existence of NLEs in diatomic chains [16–18] as well as in two-dimensional FPU systems [3, 6]. A systematic analysis of the NLE properties in two-dimensional Klein-Gordon lattices is carried out in [19]. Thus there is no doubt that by studying one-dimensional nontopological NLEs we are not restricting ourselves to exotic cases. The more complex reality will be covered. This is fundamentally different from the topological kink solutions. The reason is that the NLE solutions are not topologically induced. The only source of their existence is the nonlinearity of the underlying lattice.

All presently known theoretical approaches to describe NLEs make the assumption that the NLEs exist. Then one can proceed in the description of their properties. In this paper we want to present an approach to the problem of the existence of NLEs. We will study the simplest one-dimensional cases. As we have shown, this restriction is of no fundamental significance. We will prove several conditions when NLEs cannot exist. Thus the remaining cases are the ones one has to choose if (possibly) NLEs exist. We will use the knowledge about the interpetation of NLEs in terms of actions and angles and consider a general ansatz. Then we reduce the problem of solving coupled ordinary differential equations to a (still highly complicated) set of coupled algebraic equations. The variables are certain Fourier components. We will consider these algebraic equations as a mapping of a function defined on an n-dimensional lattice. By the definition of a NLE we show that the algebraic equations decouple in the tails of the supposed existing NLE solution. Then we analyze the decoupled mapping in the tails and calculate the eigenvalues of the linear map. We observe cases when periodic NLEs ($n = 1$) cannot exist. We prove that strictly speaking there exist no solutions for $n \geq 2$, which implies that many-frequency NLEs are unstable. Still this bare fact allows for no strict conclusion about the typical decay time of many-frequency NLEs. We relate our studies to previous work on stability analysis of NLEs.

II. FORMULATION OF THE PROBLEM

We will consider the dynamics of a simple one-dimensional Hamiltonian lattice with the following Hamiltonian:

$$H = \sum_l \left(\frac{1}{2} P_l^2 + V(X_l) + \Phi(X_l - X_{l-1}) \right) \quad . \tag{1}$$

Here P_l and X_l are canonically conjugated momentum and displacement of the lth particle, and $V(z)$ and $\Phi(z)$ are the potentials of the external field and nearest neighbor interaction, respectively. We do not consider incommensurabilities between these two potentials, thus we assume that there exists at least one ground state of Eq. (1) (minimum of the potential energy) such that without loss of generality $X_l = 0$ for this ground state. We specify the potential terms in Eq. (1) in the form of an expansion around this ground state:

$$V(z) = \sum_{k=2}^{\infty} \frac{1}{k!} v_k z^k \quad , \tag{2}$$

$$\Phi(z) = \sum_{k=2}^{\infty} \frac{1}{k!} \phi_k z^k \quad . \tag{3}$$

The NLE solution is in its general form assumed to be given by the motion of the phase space trajectory of Eq. (1) on an n-dimensional torus [13, 14]. Consequently the solution has to have the form

$$X_l(t) = \sum_{k_1,k_2,\cdots,k_n=-\infty}^{+\infty} f_{lk_1k_2\ldots k_n} \times e^{i(k_1\omega_1 + k_2\omega_2 + \cdots + k_n\omega_n)t} \quad . \tag{4}$$

The localization property of Eq. (4) is defined by the boundary condition

$$f_{lk_1k_2\ldots k_n} \mid_{l\to\pm\infty} \to 0 \quad . \tag{5}$$

Here we are excluding from the definition of a NLE localized pulses on carrier waves where the carrier wave does not decay far away from the center of the pulse. Since Eq. (4) is by assumption a solution of the equations of motion

$$\ddot{X}_l = \dot{P}_l = -\frac{\partial H}{\partial X_l} \quad , \tag{6}$$

we can insert Eq. (4) into Eq. (6) and try to solve for the Fourier coefficients on the right-hand side of 4. Using

$$\ddot{X}_l(t) = -\sum_{k_1,k_2,\ldots,k_n=-\infty}^{+\infty} y_{\vec{k}}(\vec{\omega}) f_{lk_1k_2\ldots k_n} e^{i(k_1\omega_1 + k_2\omega_2 + \cdots + k_n\omega_n)t} \quad , \tag{7}$$

$$y_{\vec{k}}(\vec{\omega}) = (k_1\omega_1 + k_2\omega_2 + \cdots + k_n\omega_n)^2 \quad , \tag{8}$$

$$\vec{k} = (k_1, k_2, ..., k_n) \quad , \quad \vec{\omega} = (\omega_1, \omega_2, ..., \omega_n) \quad , \tag{9}$$

we get Fourier series on the left- and right-hand sides of Eq. (6). The only possiblity of satisfying the obtained equation is to collect terms with equal exponents on both sides and to set the prefactors equal to each other. Then we obtain a highly complicated coupled set of algebraic equations for the Fourier coefficients and the frequencies. Because we consider nearest neighbor interaction (1) we can formally write down the resulting set of equations:

$$M_{l+1,\vec{k}} = F(\{M_{l,\vec{k}'}\},\{M_{l-1,\vec{k}''}\}) \quad . \tag{10}$$

Here we introduced a function $M_{l,\vec{k}}$ which is defined on a discrete n-dimensional lattice. The lattice is given by all combinations of $\{k_1, k_2, ..., k_n\}$ where each integer $k_{n'}$ varies from $-\infty$ to $+\infty$. We have

$$M_{l,\vec{k}} = f_{lk_1k_2...k_n} \quad . \tag{11}$$

The mapping formally derived in Eq. (10) reminds us of the well-known two-dimensional mappings which were used in order to study static kink properties, commensurate-incommensurate transitions, and breaking of analyticity [20]. We can view Eq. (10) as a first step of implementing the fruitful ideas for static topologically induced structures in the dynamical problems of nontopological NLEs in Hamiltonian lattices.

Let us study Eq. (10) in the tails of the NLE, i.e., for $l \to \pm\infty$ where Eq. (5) holds by assumption. In the generic case v_2 and ϕ_2 from Eqs. (2) and (3) will be nonzero. Then we can write down the mapping (10) explicitly. We will do it without loss of generality for $l \to +\infty$. The corresponding formula for large negative l can be obtained by substituting $l' = -l$. We find

$$M_{l+1,\vec{k}} = [\kappa_{\vec{k}}(\vec{\omega}) + 2]M_{l,\vec{k}} - M_{l-1,\vec{k}} \quad . \tag{12}$$

Here we have introduced another function on the n-dimensional discrete space which is given by

$$\kappa_{\vec{k}}(\vec{\omega}) = \frac{v_2 - y_{\vec{k}}(\vec{\omega})}{\phi_2} \quad . \tag{13}$$

Equation (12) is linear and thus every component of M in the n-dimensional discrete space decouples in this equation from all other components. Introducing

$$G_{l,\vec{k}} = M_{l,\vec{k}} - M_{l-1,\vec{k}} \tag{14}$$

we finally arrive at a two-dimensional mapping for every component of $M_{l,\vec{k}}$ which reads

$$M_{l+1,\vec{k}} = \kappa_{\vec{k}}(\vec{\omega})M_{l,\vec{k}} + G_{l,\vec{k}} + M_{l,\vec{k}} \quad , \tag{15}$$

$$G_{l+1,\vec{k}} = \kappa_{\vec{k}}(\vec{\omega})M_{l,\vec{k}} + G_{l,\vec{k}} \quad . \tag{16}$$

Let us stress that under the assumption of an existing NLE solution the linearization of the map in the tails of the NLE is arbitrarily correct, if the distance from the NLE center is large enough. This mapping has a fixed point for $M_{l,\vec{k}} = 0$ and $G_{l,\vec{k}} = 0$. It is characterized by the matrix A:

$$A = \begin{pmatrix} 1 & \kappa_{\vec{k}}(\vec{\omega}) \\ 1 & 1 + \kappa_{\vec{k}}(\vec{\omega}) \end{pmatrix} \quad . \tag{17}$$

We have

$$\det(A) = 1 \quad . \tag{18}$$

Thus the mapping (15), (16) is symplectic and volume preserving. For the eigenvalues of A we find

$$\lambda_{\pm} = 1 + \frac{\kappa_{\vec{k}}(\vec{\omega})}{2} \pm \sqrt{\left(1 + \frac{\kappa_{\vec{k}}(\vec{\omega})}{2}\right)^2 - 1} \quad , \tag{19}$$

$$\lambda_+\lambda_- = 1 \quad . \tag{20}$$

We can consider three cases:

$$\text{(a)} \quad \kappa_{\vec{k}}(\vec{\omega}) > 0 \quad : \quad 0 < \lambda_- < 1, \tag{21}$$

i.e., λ_- is real. Especially $\lambda_-[\kappa_{\vec{k}}(\vec{\omega}) \to 0] \to 1$ and $\lambda_-[\kappa_{\vec{k}}(\vec{\omega}) \to \infty] \to 0$.

$$\text{(b)} \quad \kappa_{\vec{k}}(\vec{\omega}) < -4 \quad : -1 < \lambda_+ < 0, \tag{22}$$

i.e., λ_+ is real. Especially $\lambda_+[\kappa_{\vec{k}}(\vec{\omega}) \to -\infty] \to 0$ and $\lambda_+[\kappa_{\vec{k}}(\vec{\omega}) \to -4] \to -1$.

$$\text{(c)} \quad -4 \le \kappa_{\vec{k}}(\vec{\omega}) \le 0 \quad : \quad |\lambda_+| = |\lambda_-| = 1, \tag{23}$$

i.e., $\lambda_\pm$ are complex conjugated numbers on the unit circle. Consequently in cases (a) and (b) the fixed point of the mapping is a saddle point, i.e., there exists exactly one direction (eigenvector) in which the fixed point can be asymptotically reached after an infinite number of steps. In case (c) the fixed point is a marginally stable elliptic point, i.e., starting from any direction the fixed point can never be reached after an infinite number of steps, instead the mapping will produce a (deformed) circle around the fixed point. Thus we find that case (c), (23), contradicts the localization condition (5).

III. SINGLE-FREQUENCY LOCALIZED EXCITATIONS

Let us consider $n = 1$. Then the NLE solution is periodic [cf. Eq. (4)]. Equation (13) can be simplified to

$$\kappa_{\vec{k}}(\vec{\omega}) = \frac{v_2 - k_1^2\omega_1^2}{\phi_2} \quad . \tag{24}$$

The frequencies ω_q for small-amplitude phonons around the considered ground state of Eq. (1) (where q is the wave number) are related to the parameters v_2 and ϕ_2 by

$$v_2 \le \omega_q^2 \le v_2 + 4\phi_2 \quad . \tag{25}$$

Then it follows that case (c) given in Eq. (23) is identical with

$$\text{(c)} \quad k_1^2\omega_1^2 = \omega_q^2 \quad . \tag{26}$$

We find that a single-frequency NLE (periodic localized solution) cannot exist if any multiple of its fundamental frequency equals any phonon frequency. The reason is that we cannot satisfy Eqs. (26) and (5) simultaneously because of (23).

In [13, 14] we have shown that under the assumption of the existence of a single-frequency NLE its stability with respect to small-amplitude phonon perturbations will depend on the fundamental NLE frequency. We found that if $\omega_q/\omega_1 = n/2$, $n = 0, 1, 2, ...$ then the small perturbation will grow. Consequently the NLE would collapse. Here now we find that if $n = 2k_1$ (even n) then the NLE itself could not exist. If $n = 2k_1 + 1$ (odd n) then the NLE could exist, but would be unstable against phonon perturbations.

One can interpret (26) as a definition of nonexistence bands on the ω_1-frequency axis for different k_1. Introducing a normalized frequency $\tilde{\omega}_1 = \omega_1/\sqrt{v_2}$ and normalized interaction $\tilde{\phi}_2 = \phi_2/v_2$ (only if $v_2 \neq 0$) those bands are given by

$$\frac{1}{k_1^2} \leq \tilde{\omega}_1^2 \leq \frac{1+4\tilde{\phi}_2}{k_1^2} \quad . \tag{27}$$

For any finite $\tilde{\phi}_2$ and small enough $\tilde{\omega}_1$ the nonexistence bands (27) will start to overlap. Consequently there will always be a lower bound on allowed NLE frequencies. Still some existence windows are possible in the phonon gap ($\tilde{\omega}_1 < 1$). However, with increasing $\tilde{\phi}_2$ more nonexistence bands will overlap and at the critical value $\tilde{\phi}_2^c = 3/4$ all nonexistence bands (27) overlap. For all values of $\tilde{\phi}_2 > 0$ and any value of $\tilde{\omega}_1 > 1 + 4\tilde{\phi}_2$ condition (27) is not satisfied. That means that independent of the values of the parameters $v_2 \geq 0$ and $\phi_2 > 0$ periodic NLE solutions are allowed with frequencies above the phonon band. From the above results it follows that model (1) always allows for periodic NLEs with frequencies above the phonon band. But if the model has a nonvanishing lower phonon band edge ($v_2 > 0$) then periodic NLEs with frequencies in the phonon gap are allowed if the phonon bandwidth is small enough compared to the lower phonon band edge.

Now let us make some statements about symmetries of periodic NLEs if they exist. If the frequency of the NLE is above the phonon band then it follows that $\kappa_{\vec{k}}(\vec{\omega}) < -4$ for all k_1. This corresponds to case (b) in (22). Then we have $-1 < \lambda_+ < 0$. Consequently $-1 < M_{l+1,\vec{k}}/M_{l,\vec{k}} < 0$ for all l in the tail of the NLE. Thus we find a coherent out-of-phase type of the motion of neighboring particles in the tails of the NLE solution because of Eq. (4): $-1 < X_{l+1}(t)/X_l(t) \leq 0$ if defined. If the frequency of the periodic NLE is in the phonon gap ($v_2 > 0$) things become more complicated. Namely, there will always exist a certain finite integer k_c such that for $k_1 < k_c$ it follows that $\kappa_{\vec{k}}(\vec{\omega}) > 0$, which corresponds to case (a) in (21). The corresponding Fourier components (11) would yield in-phase type of motion in the tails of the NLE solution. However, for all $k_1 > k_c$ the case (b) in (22) applies. Those Fourier components would yield out-of-phase motion. Numerical findings indicate that usually the Fourier components decay very fast with increasing k_1 [5]. Then we could expect overall in-phase type of motion. However, if the frequency ω_1 becomes smaller then it is well known that the decay in the Fourier components with increasing k_1 slows down. Thus we have to expect a complicated mixture of in- and out-of-phase type of motion.

IV. MANY-FREQUENCY LOCALIZED EXCITATIONS

Let us consider $n = 2$. Then in analogy to (26) case (c) in (23) applies if

$$v_2 \leq (k_1\omega_1 + k_2\omega_2)^2 \leq v_2 + 4\phi_2 \quad . \tag{28}$$

Now it is possible to show that there exists an infinite number of pairs of the integers (k_1, k_2) such that (28) is satisfied if the ratio ω_1/ω_2 is irrational and $v_2 \geq 0$ and $\varphi_2 > 0$ (cf. Appendix). Thus strictly speaking there exist no exact two-frequency NLEs. The proof for $n \geq 3$ is then straightforward and yields the same result. Of course this fact does not tell anything about decay times of many-frequency NLEs. It only states that many-frequency NLEs cannot exist for infinite times. It seems to be logical to assume that the decay times are sensitive to the pair of the lowest integers (k_1, k_2) for which (28) holds in the case $n = 2$. Indeed numerical simulations [13, 14] show extremely weak decay of two-frequency NLEs in Klein-Gordon chains, i.e., the characteristic decay time is several orders of magnitude larger than internal oscillation times.

V. TIME-SPACE SEPARABILITY

Recently there were reports in the literature where for systems of type (1) periodic NLE solutions with a property of time-space separability were proposed to exist [21]. In more detail this property implies the existence of a master function $G(t)$ in time such that the NLE solution can be given by

$$X_l(t) = A_l G(t) \quad , \quad A_l\mid_{l\to\pm\infty} \to 0 \quad . \tag{29}$$

Without loss of generality one can set $\max(A_l) = 1$. In terms of the Fourier components introduced in (4) ansatz (29) imposes a rather strong symmetry on the Fourier components—namely, they have to be equal to each other at different lattice sites up to a universal scaling number. If we insert (29) into the equations of motion (6) we find

$$\ddot{G}(t) = -\sum_{k=2}^{+\infty} \eta_k G^{k-1}(t) \quad . \tag{30}$$

With (2) and (3) we can specify the constants η_k:

$$\eta_k = \frac{1}{A_l}[v_k A_l^{k-1} + \phi_k\{(A_l - A_{l-1})^{k-1} - (A_{l+1} - A_l)^{k-1}\}] \quad . \tag{31}$$

If η_k in Eq. (31) depended on l then the differential equation for the master function $G(t)$ in Eq. (30) would yield different solutions for different lattice sites (cf., e.g., [22]). Then we contradict the original ansatz (29). Thus we have to assume that η_k in (31) is independent of l. Hence we generate a set of two-dimensional mappings for the vector (A_l, A_{l-1}) in Eq. (31) for different k.

Let us show that generically we cannot satisfy all those mappings. For that we consider a Klein-Gordon lattice, i.e., $\phi_k = 0$ for $k \geq 3$, at least one v_k is nonzero for $k \geq 3$. Then we consider Eq. (31) for that specific k:

$$\eta_k = v_k A_l^{k-2} \quad , \quad k \geq 3 \quad . \tag{32}$$

From (32) it would follow that $A_l = 1$ for all l in contradiction to (29). Thus we would have to conclude that either no NLEs exist in Klein-Gordon lattices or that they do not obey separability property (29). The existence of periodic NLEs in various Klein-Gordon systems is verified numerically with very high probability (i.e., currently periodic NLEs can be generated without any measurable energy loss over 10^6 time periods of the internal NLE oscillation, cf. Sec. VI). Consequently the ansatz (29) is restricted to a certain subclass of systems which excludes the Klein-Gordon systems. Now let us consider any system such that for only (or at least) one integer k we have $v_k = \phi_k = 0$. Let us assume that we have periodic NLE solutions which satisfy Eq. (29). Perturbing this system with any small but finite $v_k \neq 0$ we can again consider the mapping for that k and yield (32). Consequently no NLE solution would be allowed. Thus the separability ansatz (29) becomes a real exotic property.

There is one case when we can at least expect that Eq. (29) holds. Namely, when we have to satisfy only one mapping of the type (31). This can happen, e.g., if $v_k = 0$ for all k and $\phi_{k_0} \neq 0$ for $k_0 \leq 4$ and k_0 even and $\phi_k = 0$ for all $k \neq k_0$. One can prove that if Eq. (31) is rewritten for that specific case in terms of a mapping of the two-component vector $(A_l, A_l - A_{l-1})$ then the mapping will be nonconservative (it does not preserve phase volume). A numerical test for $k_0 = 4$ yields that a periodic NLE solution can be found for $\eta_{k_0} = 9.584\,377\,377\,631\,4\ldots$. The amplitudes for that solution read $\ldots 0.004\,795, -0.165\,787\,9, 1, -1, 0.165\,787\,9, -0.004\,795, \ldots$. First we notice that indeed for such special systems it can be possible to generate a NLE solution with time-space separability property (29). However, our result also indicates that even for such a highly nonlinear model (no linear dispersion) the NLE if it exists has no compact structure, i.e., the amplitudes A_l are not exactly zero outside a finite volume of the solution. That fact can also be observed by looking at (31). If outside of a finite volume of a solution all amplitudes would be equal to zero, by inverting the mapping we would generate zeros for all amplitudes in the excluded finite volume, thus contradicting the ansatz that at least one amplitude is equal to 1. As a consequence the claimed compacton structure of a periodic NLE solution in [21] is wrong and based on a simple calculation error.

VI. THE DECAY OF SINGLE-FREQUENCY NLES IN THE TAILS

Let us consider an existing periodic NLE for system (1) with $v_2 > 0$, $\phi_2 > 0$. Then in the tail of the NLE (without restriction for large positive l) every Fourier component obeys a two-dimensional mapping given in (15), (16). The eigenvalue describing the decay is given by (19), (24). Then the decay of every Fourier component will be governed by an exponential law $\sim [\mathrm{sgn}(\lambda)]^l e^{\ln|\lambda| l}$. The absolute value of λ will depend on the number k of the Fourier component. For $l \to \infty$ only the Fourier component with $|\lambda|$ closest to one will be present, i.e., all other Fourier components will decrease exponentially fast compared to the remaining one. The answer to the question which Fourier component "survives" depends on the frequency ω_1 and on the parameters v_2 and ϕ_2. Only if ω_1 is above the phonon band then can we state that the "surviving" Fourier component is that with $k = 1$.

In the following we will formulate two predictions for single-frequency NLEs in order to test them in a given realization. The first prediction was already formulated above—if an assumed periodic NLE (characterized by its fundamental frequency ω_1) exists, the amplitude decay in the tails of the NLE (i.e., where the nonlinear terms in the equations of motion can be neglected) is governed by an exponential law with exponent $\ln|\lambda|$. Let us consider the case of a ϕ^4 chain, i.e., $V(z) = z^2 - z^3 + 0.25z^4$ and $\Phi(z) = 0.5Cz^2$. Consequently we have $v_2 = 2$, $\phi_2 = C$. Periodic NLEs were investigated in [13, 14] on finite time scales for the case $C = 0.1$. We use a particular realization with energy $E = 0.256$ (for details on the numerics the reader should consult the original work [13, 14]). The initial conditions on the lattice (3000 particles) are found from analyzing the elliptic fixed point of a reduced problem [14]. The frequency of the periodic localized object is found to be $\omega_1 = 1.177$ (cf. Fig. 10 in [14]). After a waiting time of $T = 3 \times 10^5$ the energy stored in five particles around the excitation center is still $E(T) = 0.256$. There is absolutely no drift (radiation) observable. The symmetric amplitude distribution in this assumed NLE solution is shown in Fig. 1 in a semilogarithmic plot (open squares). An evaluation of the eigenvalues corresponding to the different Fourier components [cf. Eqs. (19)–(24)] reveals in this case that the eigenvalue with absolute value closest to one is given for $k = 1$ and reads $\lambda = 0.124\,65$ ($\kappa_1 = 6.1467$). Consequently in the tail of the solution (where the nonlinear terms in the equations of motion can be neglected) we find an exponential amplitude decay with exponent $\log_{10}|\lambda| = -0.904$. The dashed line is this prediction of the exponential decay. Note that in the semilogarithmic plot in Fig. 1 this decay law appears as a straight line. This line fits the measured amplitude decay down to amplitudes of 10^{-3}. The deviations for smaller amplitudes (farther away in the tail) are due to the fact that the numerical realization of the NLE solution is always accompanied by the existence of phonons. The phonons with

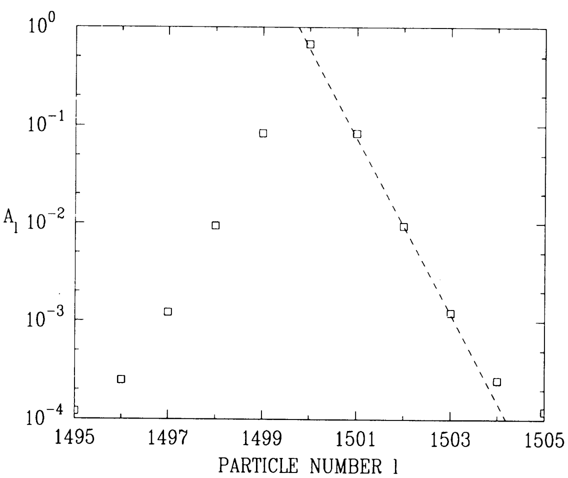

FIG. 1. Amplitude distribution for a localized state in the Φ^4 chain (cf. text). Open squares—numerical result. Dashed line—predicted decay law (cf. text).

nearly zero group velocities (wave numbers close to band edges) are practically not moving. These small phonon contributions increase (additively, as has to be expected in a linearizable tail of a NLE) the amplitudes of the particles in the NLE solution. We have no knowledge of any result in the literature, where from the measurement of the frequency of an assumed NLE solution the amplitude decay in the NLE tails was successfully predicted.

The second prediction we wish to formulate is, that if the NLE frequency ω_1 is restricted to be in the nonzero gap of the phonon spectrum, then there exists a nonzero value of $\omega_1^{(m)}$ such that the exponential decay in the NLE tails will be weaker for all other frequencies ω_1 (still belonging to the gap). Let us explain why this statement follows out of the previous considerations. First the frequency ω_1 has to be larger than the phonon bandwidth—otherwise one (or more) multiple of ω_1 will always lie in the phonon band. Secondly, if ω_1 is slightly below the lower phonon band edge, then the decay will be very weak. Lowering the ω_1 we increase the decay exponent, but since $2\omega_1$ is coming closer to the upper phonon band edge, there will be a certain frequency when the decay in the tails will be governed by the second harmonic rather than the first harmonic of ω_1. Let us calculate $\min[1-|\lambda(\kappa_k)|]$ with $|\lambda(\kappa_k)| \leq 1$ and the parameters of the above introduced ϕ^4 chain for different ω_1. The result is shown in Fig. 2. We see indeed that there is a maximum in the decay exponent in this given example for $\omega_1^{(m)} = 0.938$. As it can be observed from Fig. 10 in [14], there are two NLE energies $E_1 = 0.336$ and $E_2 = 0.85$ which correspond to this particular frequency $\omega_1^{(m)}$. The prediction is thus that by varying the energy of the periodic NLEs, in a simulation one should observe maximum amplitude localization at these two energies E_1, E_2. From the numerical runs reported in [14] we can calculate a normalized amplitude entropy σ_a which measures the amplitude distribution of the solution. It is defined in analogy to the energy entropy which is defined in [14]: $\sigma_a = -1/[\ln(N)] \sum_l a_l \ln a_l$ with $a_l = A_l / \sum_l A_l$. Here A_l is the amplitude of particle l. From the definition we have $0 < \sigma_a < 1$. Maximum localization corresponds to a minimum of the normalized entropy. σ_a as a function of the NLE energy is shown in Fig. 3 (filled triangles and solid line). The predicted positions of the minima of $\sigma_a(E)$ at E_1, E_2 are given by vertical dashed lines. The predicted positions of the minima agree with the measured ones within the energy grid of the numerical experiment.

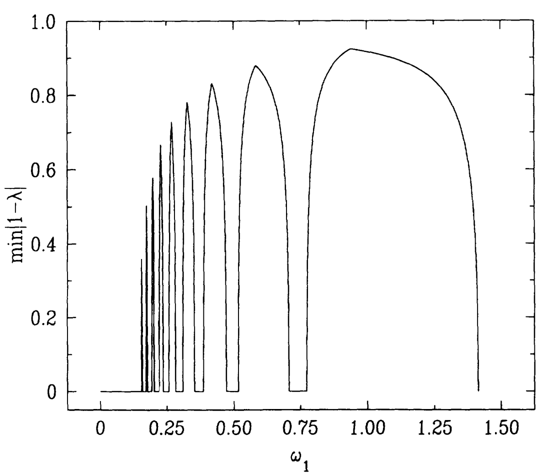

FIG. 2. Minimum of the distance of the absolute value of eigenvalue λ from 1 as a function of the fundamental frequency ω_1. Here $|\lambda| \leq 1$, minimization is obtained with respect to all Fourier components for a Φ^4 chain with parameters given in the text.

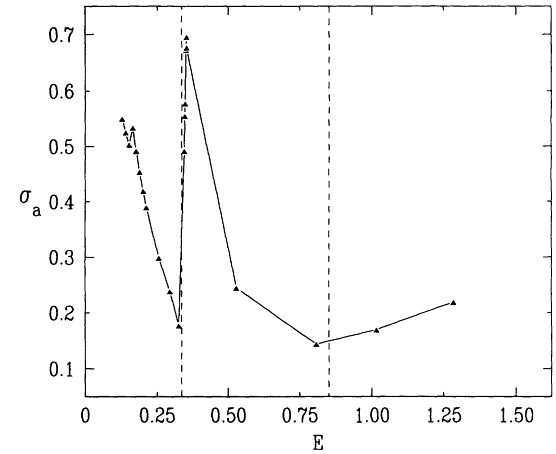

FIG. 3. Normalized amplitude entropy σ_a versus NLE energy for a Φ^4 chain (cf. text). Filled triangles—numerical result. Solid line connects the triangles and serves as a guide to the eye. Dashed vertical lines—predicted positions of minima of σ_a (cf. text).

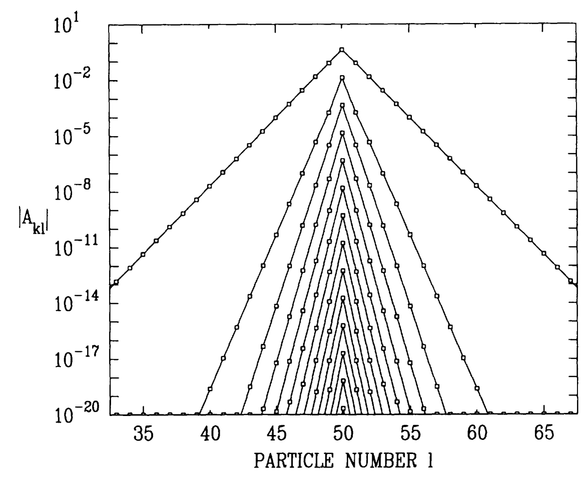

FIG. 4. Numerical solution for the Fourier components of the periodic NLE of a system with $v_2 = 1$, $v_4 = -1$, $\phi_2 = 0.1$, $N = 100$, $\omega_1 = 0.8$ (cf. text). The absolute values of the components A_{kl} are shown as functions of the lattice site l in a window of 30 lattice sites around the NLE center. The open squares are the actual results. The lines are guides to the eye and connect components with same Fourier order k. k increases from top to bottom as $k = 1, 3, 5, 7, ..., 23, 25$. Fourier components for even k are zero because of the symmetry of the potential.

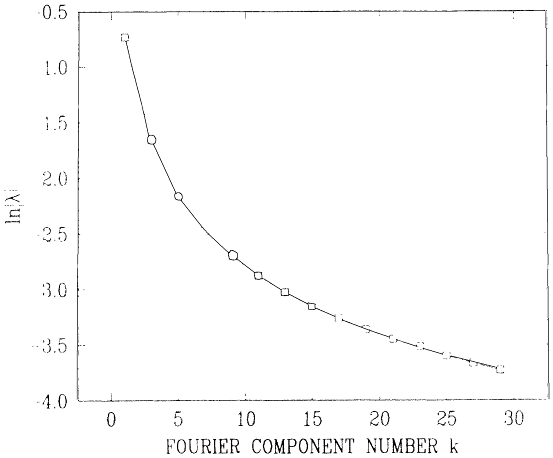

FIG. 5. Slopes of the lines in Fig. 4 as a function of k (correspond to the exponents of the decay of the corresponding Fourier components, cf. text) are shown as open squares. The solid line connects the points of the theoretical prediction using the eigenvalues of the linearized map (cf. text).

In order to demonstrate the usefulness of the above considered spatial decay laws, we have implemented a numerical method in order to solve the *full nonlinear* equations for the Fourier coefficients (10) for a periodic NLE ($n = 1$) on a finite lattice. We have chosen $v_2 = 1$, $v_4 = -1$, $v_{k\neq 2,4} = 0$, $\phi_2 = 0.1$, $\phi_{k\neq 2} = 0$, and a system size of 100 particles with periodic boundary conditions. The NLE frequency was chosen to be below the phonon band: $\omega_1 = 0.8$. The resulting Fourier coefficients were computed on every lattice site with a maximum multiple of the fundamental frequency $|k|_{\max} = 30$ and a numerical error of 10^{-20}. The result is shown in Fig. 4 for 30 lattice sites around the NLE center in a semilogarithmic plot. Clearly a k-dependent exponential decay of every Fourier component is found. Moreover in Fig. 5 we plot the measured exponents (slopes) as found from the numerical solution and compare them to the theoretical prediction. The agreement is very good.

What happens if $v_2 = 0$ and $\phi_2 = 0$? We can give a particular answer for the special case $\phi_4 \neq 0$ and all other coefficients in (2), (3) being zero. This case was already discussed in the preceding section. If we know that a periodic NLE exists we can consider the mapping (31). We linearize the map near the saddle fixed point and find in leading order a decay of the amplitudes according to the law $e^{-a \exp bl}$ where a and b are positive numbers which depend on the parameters of the model Hamiltonian.

VII. CONCLUSION

Nonlinear localized excitations might exist in nonlinear lattices for infinite times (i.e., they can be exact solutions of the equations of motion) if they are periodic in time and all multiples of the fundamental frequency are outside the phonon band. This is only possible because of the discreteness of the underlying lattice. A continuum system would have no upper phonon band edge, thus resonance would always be possible. Exceptions are classes of nongeneric systems where the resonance condition holds but the coupling between the NLE and the phonons is exactly zero.

Let us note that we have not shown that periodic NLEs *will* exist on a given nonlinear lattice. We have restricted the possibilities of NLE solutions to time-periodic NLEs.

If the NLE solution is described by two or more fundamental frequencies then there will always be resonance with phonons and thus those solutions cannot exist for infinite times, i.e., they are not exact solutions of the equations of motion. Nothing can be said up to now about the lifetimes of such solutions. Numerical testing shows that lifetimes can be very large compared to internal oscillation times. If one considers nongeneric lattices without linear dispersion (phonons) then many-frequency NLEs might be exact solutions of the equations of motion.

Space-time separability in the NLE solution can appear only in very nongeneric cases. The construction of mappings for Fourier coefficients in higher-dimensional Hamiltonian lattices seems to be more complicated but this is a technical question. The construction of the existence conditions for NLEs indicates that one can generalize them for higher dimensions too.

Let us make some comments on the results represented in this paper. First we have assumed that the NLE solution (if it exists) is given by a regular motion on a torus in the phase space of the system (discrete spectrum). It is very hard to believe that NLE solutions can exist if the corresponding orbit belongs to a stochastic part of the system's phase space (continuous spectrum). Assuming the NLE solutions we search for are regular, all the subsequent steps in the presented analysis are free from any simplifications, approximations, or conjectures. We have formulated the leading order amplitude decay of an assumed NLE solution in its tails. We were thus able to formulate two nontrivial predictions and test them by comparing to numerical experiments.

Recently it was shown by using the properties of map (10) that the existence of NLE solutions is equivalent to finding a common point of two separatrix manifolds of the nonlinear map [27]. It was argued that the corresponding task is not overdetermined and should lead to a discrete set of solutions. Moreover in the case of an anharmonic Fermi-Pasta-Ulam chain with homogeneous potential $v_k = 0$, $\phi_{2m} = 1$, $\phi_{k\neq 2m} = 0$ (where m is any positive integer with $m \geq 2$) the existence of time-periodic NLEs could be strictly proved [27].

Since the presented analysis was carried out in the tails of the NLE solution (where the corresponding mappings can be linearized) the legitimate question arises of why we do not have NLE solutions in a purely harmonic lattice. The reason for the nonexistence of a localized solution in such a linear lattice is that the two separatrix manifolds of the saddle fixed point never cross, because the eigenvectors of the fixed point uniquely define the positions of the two separatrix manifolds. In a nonlinear system, inverting the discrete map (i.e., starting in the tail of an assumed existing NLE and iterating towards the center of the NLE) the increase of the amplitudes (or Fourier coefficients) will increase the contributions coming from the nonlinearity. These nonlinearities will be the reason for the crossing of the separatrix manifolds. We wish to emphasize that still these arguments cannot be considered as a proof of the existence of NLEs. They provide the possible source of the NLE existence in the framework of the presented approach. The aim of the present work was to analyze the NLE properties in the tails assuming the NLE existence. The results obtained restrict possible NLE solutions to time-periodic solutions.

Recently MacKay and Aubry have carried out a proof of existence of time-periodic NLEs for Hamiltonian networks of weakly coupled oscillators [28]. This strict proof remarkably incorporates Hamiltonian lattices with and without disorder. Consequently one can see that (at least in the limit of weak coupling) the NLEs in a nonlinear lattice are continuously connected with localized modes of, say, a harmonic lattice with defects. These results should once and forever make it clear that a harmonic lattice without defects is a very isolated system, and one should never use it as a reference system in order to judge results of nonlinear theories. In the present work the proof of MacKay and Aubry corresponds to the case $v_k \neq 0$, $\phi_k \ll v_2$. According to [28] the spatial decay of NLEs is at least exponential, which can be specified to be strictly exponential in the present work without the requirement of weak coupling. Together with the strict proof of NLE existence in the mentioned anharmonic FPU chain [27] we thus have an analytical basis of the existence of NLEs in a broad class of systems.

We were able to construct a mapping for the NLE solutions because of our knowledge about their proposed dynamical behaviour. This knowledge comes from the interpretation of the NLE solutions as motion of phase space points on tori in the phase space. The resulting mapping is an algebraic problem and can be considered as a task for itself. Here we meet numerous results for approximate NLE solutions which use the rotating wave approximation (RWA) [1, 23, 24, 5, 18]. Within the RWA all Fourier components higher than a certain hand-chosen order are set to zero. The resulting algebraic equations can be either solved self-consistently or by means of useful iteration procedures. Only periodic NLEs were considered up to now.

It is interesting to note that recently a combination of the lowest RWA order (taking into account only the lowest Fourier component) was reformulated into a mapping [25]. It would correspond to the mapping for the amplitudes of the NLE solution in the present work under the assumption of time-space separability.

The fact that the existence of NLEs seems to be a generic property of (nonlinear) Hamiltonian lattices implies that either experimental realizations of NLEs can be found with probability 1 or that the considered model classes are useless in describing reality. This promises some intriguing questions for the future.

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APPENDIX

Let us prove that if a and b are two real numbers such that

$$0 \leq a < b \tag{A1}$$

and ω_1 and ω_2 are two real numbers such that

$$0 < \omega_1 < \omega_2 \tag{A2}$$

and the ratio ω_1/ω_2 is irrational, then there always exists an infinite number of pairs of integers (k_1, k_2) such that

$$a \leq | k_1\omega_1 + k_2\omega_2 | \leq b \quad . \tag{A3}$$

Let us introduce

$$\tilde{a} = \frac{a}{\omega_2} \quad , \quad \tilde{b} = \frac{b}{\omega_2} \quad , \quad \xi = \frac{\omega_1}{\omega_2} \quad . \tag{A4}$$

Then (A3) is equivalent to

$$\tilde{a} \leq | k_1\xi + k_2 | \leq \tilde{b} \quad . \tag{A5}$$

Let us choose the numbers $\tilde{c}$ and $\tilde{d}$ such that

$$\tilde{a} < \tilde{c} < \tilde{b} \quad , \quad \tilde{d} = \min((\tilde{c} - \tilde{a}), (\tilde{b} - \tilde{c})) \quad . \tag{A6}$$

We can consider an arbitrary integer N such that

$$N > \frac{1}{n\tilde{d}} \quad , \tag{A7}$$

where $n = 1, 2, 3, \ldots$ and is fixed. Then it follows that there exists at least one pair of integers (k_1^0, k_2^0) with $1 \leq k_1^0 \leq N$ such that

$$0 < \mu < \frac{1}{N} \quad , \quad \mu = | k_1^0\xi + k_2^0 | \tag{A8}$$

(cf. [26]). If we denote by m the integral part of $\tilde{a}/\mu$:

$$m = \left[\frac{\tilde{a}}{\mu}\right] \tag{A9}$$

we find

$$\tilde{a} \leq (m + n')\mu \leq \tilde{b} \quad , \quad 1 \leq n' \leq n \quad . \tag{A10}$$

Thus our condition (A3) can always be fullfilled if we choose

$$k_1 = (m + n')k_1^0 \quad , \quad k_2 = (m + n')k_2^0 \quad . \tag{A11}$$

Since there is no restriction on the integer n in (A7) it follows from (A11) that we generate an infinite number of pairs (k_1, k_2) which satisfy our inequality (A3).

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