

Localized excitations in two-dimensional Hamiltonian lattices

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We analyze the origin and features of localized excitations in a discrete two-dimensional Hamiltonian lattice. The lattice obeys discrete translational symmetry, and the localized excitations exist because of the presence of nonlinearities. 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. This work is an extension of previously published results on vibrational localization in one-dimensional nonlinear Hamiltonian lattices [Phys. Rev. E **49**, 836 (1994)]. Thus we confirm earlier suggestions about the generic property of Hamiltonian lattices to exhibit localized excitations independent of the dimensionality of the lattice.

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I. INTRODUCTION

In this contribution we will deal with vibrational localization in Hamiltonian lattices *without* any kind of disorder. We consider a solution of a set of coupled ordinary differential equations (CODEs) of an underlying Hamiltonian system. The localization property of the solution implies the solution to be essentially zero (constant) outside a certain finite volume of the system. Inside the specified volume the solution has some oscillatory time dependence. The absence of disorder implies the existence of certain discrete (CODE) translational symmetries of all possible solutions.

Usually vibrational localization can be produced by considering a lattice with a defect (diagonal or off-diagonal disorder) [1]. Another well known possibility is to consider lattices with more than one ground state (global minima of the potential energy) and static kinklike distortions of the lattice. The presence of the kinklike static (stable) distortion of the lattice breaks the discrete translational symmetry as in the case of a defect. This is the key ingredient to get localized vibrations (localized modes) centered around either the defect or the kinklike distortion [1]. It is worthwhile to mention that the existence of kinklike distortions implies that the underlying Hamiltonian lattice is nonlinear.

However, it was known for a long time that special partial differential equations admit breather solutions. These breather solutions are exact localized vibrational modes, which require neither disorder nor kinks. In the case of the sine-Gordon (SG) equation the *tangent* of the breather solution is given by a product of space-dependent and periodic time-dependent functions [2].

The SG system has a phonon band with a nonzero lower phonon band edge (the upper band edge is not present since its finiteness would imply the discreteness of the system). The fundamental frequency of the breather lies in the phonon gap below the phonon band. The representation of the inverse tangent of the periodic time master function in a Fourier series shows up with contributions from higher harmonics of the fundamental frequency. These higher harmonics will certainly lie in the phonon band. The stability of the breather solution in such a partial differential equation will depend on some orthogonality properties between the breather (higher harmonics) and the extended solutions (phonons) [3]. The fulfilling of all these orthogonality relations seems to be connected to the fact that the SG equation is integrable, i.e., admits an infinite number of conservation laws. Thus it appears logical that the SG breather solutions survive only under nongeneric perturbations of the underlying Hamiltonian field density [4, 5]. Indeed efforts to find breather solutions in partial differential equations of the Klein-Gordon type (i.e., closely related to the SG case) failed, e.g., for the Φ^4 equation [6]. The Φ^4 equation is not integrable.

Consider now instead of a partial differential equation a Hamiltonian lattice. It will have at least one ground state. Generically the expansion of the potential energy around the ground state yields in lowest order a harmonic system and thus phonons. However, the phonon band will now have a finite upper band edge. Thus we can imagine the creation of a breatherlike localized state with its frequency either above the phonon band or even in a nonzero gap below the phonon band. In the first case there will never be resonances between any harmonics of the time function governing the evolution of the discrete breather and phonons. In the second case we can again avoid resonances by a proper choice of the fundamental frequency and the requirement that the phonon band width is smaller than the gap width. Hence we seem to lose the necessity to satisfy an infinite number of orthogonality relations as in the continuum case. That could mean in turn that the existence of discrete breather so-

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lutions will not be restricted to a subset of nongeneric Hamiltonian lattices.

Indeed over the past six years there have been several reports on the existence of discrete breathers in various one-dimensional nonintegrable Hamiltonian lattices of the Fermi-Pasta-Ulam type and the Klein-Gordon type [7–14]. Unsurprisingly one will find no rigorous derivation of the discrete breather solution in those reports; it would be better to say that numerical results and several approximate analytical results strongly imply the existence of discrete breathers in one-dimensional nonintegrable Hamiltonian lattices.

Recently a careful study of the above mentioned system classes revealed an understanding for the phenomenon of discrete breathers in terms of phase space properties of the underlying system [15–18]. We will call these discrete breathers *nonlinear localized excitations* (NLEs). It was shown that the NLE solution can be reproduced with very high accuracy considering the dynamics of a reduced problem. In the reduced problem one keeps the few degrees of freedom which are essentially involved in the NLE solution of the extended system. It turned out that the NLE solutions correspond to regular trajectories in the phase space of the reduced problem. These regular trajectories belong to a certain compact subpart of the phase space which can be called regular island. The NLE regular island is separated by a separatrix from other regular islands which correspond to extended states in the full system. Trajectories of the reduced problem on the separatrix itself as well as in a certain energy-dependent part of the phase space surrounding it are chaotic because the full system as well as the reduced problem are nonintegrable. The whole emerging picture we will call the local integrability scenario.

As it follows from that scenario, single-frequency NLEs correspond to the excitation of one main degree of freedom, which can be characterized by its action J_1 and frequency $\omega_1 = \partial H / \partial J_1$ [16]. Many-frequency NLEs correspond to the excitation of several secondary degrees of freedom, which can be characterized by their actions J_m , $m = 2, 3$, and frequencies $\omega_m = \partial H / \partial J_m$ [16]. Stability of the NLEs in the infinite lattice environment can be studied with the help of mappings. A certain movability separatrix can be defined by $\omega_3 = 0$. This separatrix separates the phase space into stationary NLEs (i.e., the center of energy oscillates around a given mean position) and movable NLEs (i.e., the center of energy can travel through the lattice) [18].

On the basis of the local integrability scenario it was recently possible to prove the generic existence of NLE solutions in a one-dimensional nonlinear lattice with *arbitrary* number of degrees of freedom per unit cell and *arbitrary* (still finite) interaction range [19]. Moreover a rigorous proof was given that periodic NLE solutions *do exist* in a class of Fermi-Pasta-Ulam lattices [19].

From the local integrability scenario it follows that there are no principal hurdles in going over to higher lattice dimensions (by that we refer to the topology of the interactions rather than the number of degrees of freedom per unit cell). Indeed the NLEs are described

through *local* properties of the phase space of the lattice and no topological requirements on the potential energy are necessary to allow for NLE existence. This is very different compared to the well known topologically induced kink solutions, for which the one-dimensional lattice is an analytical requirement. Only under very special constraints can one discuss kinklike solutions in lattices with higher dimensions. Thus the NLE existence occurs to be a *generic* property of a nonlinear Hamiltonian lattice. Indeed a few numerical studies on NLEs in two-dimensional Fermi-Pasta-Ulam lattices showed that NLEs exist there [20, 21].

The purpose of this contribution is to apply the successful local integrability picture from one-dimensional lattices [15, 18] to two-dimensional lattices. We will show that we indeed again find NLE solutions (which are somewhat richer in their properties compared to the one-dimensional case) which are quantitatively describable with a reduced problem. We will show this by comparing the phase space properties of the full lattice and the reduced problem. We present a stability analysis of the NLEs as well as a scheme to account for NLE properties. Finally we present arguments about the statistical relevance of the NLEs in the considered lattices at finite temperatures. Thus we are able to show the correctness of our general approach to vibrational localization in nonlinear Hamiltonian lattices and of viewing NLEs as generic solutions in nonlinear discrete systems.

The paper is organized as follows. In Sec. II we introduce the model and briefly review the properties of NLEs in one dimension. In Sec. III examples of NLE solutions in two dimensions are presented. Then we define the reduced problem for the two-dimensional system; its phase space structure is compared to the corresponding part of the phase space of the whole lattice. A stability analysis is described and different evolution scenarios of NLEs are explained. Section IV is used for a discussion of the results.

II. MODEL: SOLUTIONS IN ONE DIMENSION

We study the dynamics of lattices with one degree of freedom per unit cell and nearest neighbor interaction. The general Hamiltonian is given by

$$H = \frac{1}{2} \sum_{\vec{R}} P_{\vec{R}}^2 + \sum_{\vec{R}} V(X_{\vec{R}}) + \frac{1}{2} \sum_{\vec{R}} \sum_{\vec{N}} \Phi(X_{\vec{R}} - X_{\vec{R}'}) . \quad (1)$$

Here $P_{\vec{R}}$ and $X_{\vec{R}}$ are canonically conjugated momentum and displacement of the particle in the unit cell characterized by the d -dimensional lattice vector \vec{R} . The d components of \vec{R} are multiples of the lattice constant $a = 1$. The interaction and on-site potentials $\Phi(z)$ and $V(z)$ are defined through

$$\Phi(z) = \sum_{n=2}^{\infty} \phi_n \frac{z^n}{n!} , \quad (2)$$

$$V(z) = \sum_{n=2}^{\infty} v_n \frac{z^n}{n!} . \quad (3)$$

\mathcal{N} in (1) means summation over all nearest neighbor positions \vec{R}' with respect to \vec{R} . Hamilton's equations of motion for the model are

$$\dot{X}_{\vec{R}} = P_{\vec{R}} \quad , \quad \dot{P}_{\vec{R}} = -\frac{\partial H}{\partial X_{\vec{R}}} \quad . \quad (4)$$

Thus we exclude from our consideration cases with (i) more than one degree of freedom per unit cell and (ii) a larger interaction range. The reasons for that are pragmatic—it will become too difficult at the present stage to present a careful study for the excluded cases. We mention the numerical investigations of one-dimensional chains with two degrees of freedom per unit cell in [22, 23] and some qualitative thoughts in [24] about long range interactions, where no indications of a change of the NLE existence properties are found.

Let us briefly review the results for NLE properties in the one-dimensional case. They are reported for two major subclasses of (1)–(3): the Klein-Gordon lattices [15–17] and the Fermi-Pasta-Ulam lattices [18]. In the case of Klein-Gordon lattices one drops the nonlinearities in the interaction $\phi_2 = C \neq 0$, $\phi_{n>2} = 0$ and allows for nonlinearities to appear in the onsite potentials. Examples are the Φ^3 model [$V(z) = 1/2z^2 + 1/3z^3$], the Φ^4 model [$V(z) = 1/4(z^2 - 1)^2$], and the sine-Gordon model [$V(z) = \cos(z)$]. In the case of Fermi-Pasta-Ulam (FPU) lattices one drops the on-site potential $V(z) = 0$ and allows for nonlinearities to appear in the interaction $\Phi(z)$. In a convenient notation we will refer to them as FPU klm models, where k, l , and m are positive integers indicating the corresponding nonvanishing power coefficients in (3). The Klein-Gordon systems have a nonzero lower phonon band edge frequency (if $v_2 \neq 0$) whereas the Fermi-Pasta-Ulam systems have a zero lower phonon band edge frequency. Consequently the FPU models exhibit total momentum conservation and show up with a zero frequency Goldstone mode, in contrast to the Klein-Gordon lattices. Stable periodic (in time) NLEs can be created in nearly all cited systems with frequencies outside the phonon band (below or above for the Klein-Gordon systems, above only for the FPU systems). The lowest NLE energy is nonzero, i.e., there is a gap in the density of states of NLEs for energies lower than the threshold energy. There can be gaps at higher energies too, depending on resonance conditions between the NLE frequency and the phonon frequencies. To allow for stable NLEs with frequencies below the phonon band for Klein-Gordon systems one has to require that the phonon band width is smaller than the phonon gap width. One can understand the existence of a gap in the NLE density of states by an approximate method to account for the NLE frequency. It consists out of constructing an effective nonlinear one-particle potential. The energy of a particle moving in this effective potential is the NLE energy and the fundamental frequency of its oscillation is the NLE frequency. For small amplitude oscillations (small energies) the frequency will lie always inside the phonon band of the corresponding lattice. Increasing the amplitude (energy) will change the frequency because of the nonlinearity. Depending on the type of the effective potential the frequency can decrease or increase. At

a certain value of the amplitude (energy) the frequency leaves the phonon band; thus the NLE becomes a stable excitation. This is also a very simple guide to the prediction of the existence or nonexistence of NLEs in nonlinear lattices. There will be no stable NLEs allowed to exist in systems with, e.g., a zero lower phonon band edge and an effective potential of the defocusing type, i.e., where the frequency will always decay with increasing amplitude (energy). Instructive examples are the Toda lattice and the FPU 2β lattice.

Because of the localization character of the NLE solutions essentially only a finite number of particles are involved in the motion. Thus it is possible to define a *reduced problem* [16]. It consists of defining a finite volume around the NLE center. All particles inside the finite volume are involved in the NLE solution; particles outside essentially should not be involved. There is an uncertainty in the definition of the finite volume. It comes from the fact that the NLE solutions are not compact, i.e., strictly speaking they incorporate an infinite number of particles (degrees of freedom) [25]. But a sharp exponential decay of the amplitudes starting from the center of the NLE provides a good finite volume choice in many cases. Since the finite volume (reduced problem) consists out of a finite number of degrees of freedom, it becomes easier to analyze its phase space properties. As it was shown in [16], there exist regular islands in the phase space of the reduced problem. These regular islands are separated by stochastic layers (destroyed regular motions on and near separatrices) from each other. The motion in each of the regular islands appears to be confined to a torus of corresponding dimension. Certain islands can be labeled NLE islands. Periodic orbits (elliptic fixed points in corresponding Poincaré mappings) from these NLE islands appear to be (nearly) exactly the periodic NLE solutions from the full system. The surprise came when it was shown that the quasiperiodic orbits surrounding the periodic one correspond to many-frequency NLEs in the full system [15, 16]. Although a stability analysis shows that these many-frequency NLEs are strictly speaking unstable (i.e., they cannot exist for infinite times) [25], it turned out that their energy radiation rate can be very weak, such that the lifetimes of these many-frequency NLEs can become several orders of magnitude larger than the typical internal periods. In numerical experiments more than five orders of magnitude were easily found [16]. The lifetime of the many-frequency NLEs will increase to infinity if one chooses quasiperiodic orbits which are closer and closer to the periodic orbit (the periodic NLE).

Other regular islands did not yield NLEs in the full system. The same can be said about the orbits in the stochastic layer. The reason for that is the resonance of the fundamental frequencies in those regular islands with the phonon frequencies. Motion in the stochastic layer is chaotic; thus frequency spectra are continuous rather than discrete. Consequently, generically there is always overlap with the phonon frequencies and thus strong energy loss of the finite volume. We also mention interesting long-time evolutionary scenarios for many-frequency NLEs as described in [16].

The clear correspondence between regular islands in the reduced problem and NLE solutions in the full system allows for a deep understanding of the NLE phenomenon on one side. On the other side it opens possibilities to apply the apparatus of nonlinear dynamics to explore NLE properties. That was done in [18] to study the movability properties of NLEs.

In the following we will apply the same procedure to characterize NLE solutions in two-dimensional systems. The success of our study will have several impacts. First it will be a proof of the conjecture that the NLE existence is not a specific one-dimensional solution such as, e.g., the kinks. This conjecture was formulated on the basis of the local integrability picture [16] as described above. Thus we strengthen the whole local integrability picture. Second, establishing NLE solutions in two-dimensional lattices undoubtedly will increase the interest in the overall phenomenon because of the variety of physical applications in contrast to the one-dimensional case. Moreover by proving the conjecture about the unimportance of the dimensionality of the lattice with respect to the NLE occurrence also three-dimensional applications become of potential interest.

III. THE TWO-DIMENSIONAL CASE

A. Model specification: Numerical details

As an example we choose the ϕ^4 lattice in two dimensions, i.e., $V(z) = 1/4(z^2 - 1)^2$, $\Phi(z) = 1/2Cz^2$, $\vec{R} = (l, m)$ with $l, m = 0, \pm 1, \pm 2, \dots$ [cf. (1)–(3)]. The two ground states of the system are given by $X_{\vec{R}} = \pm 1$. The model has a phase transition at a finite temperature T_c , which is of no further concern here since we are studying properties of single excitations above the ground state (i.e., because of the localized character of the solutions at effectively zero temperature). The parameter C specifies the “discreteness” of the system, i.e., the ratio of the phonon band width to the phonon gap width. Since we are interested in vibrations localized on a few particles, it is reasonable to compare the onsite potential energy $[V(z)]$ to the spring energy $[\Phi(z)]$ of a given particle when it is displaced relative to its nearest neighbors. As it was shown in [16], besides the interaction parameter C the energy (per particle) becomes a second significant parameter in order to choose a reasonable ratio between the two components of the potential energy. One can easily take over the results from [16] if one rescales the parameter C there by multiplying it with 2 (because in the cited one-dimensional case the coordination number was 2 compared to 4 in the two-dimensional case). Thus a choice of $C = 0.05$ turns out to be a case of intermediate interaction for not too large energies, i.e., the on-site potential energy is of the same order as the interaction potential energy.

The dispersion relation for small amplitude phonons (small amplitude oscillations around either ground state) is given by

$$\omega_{k_x, k_y}^2 = 2 + 4C \left[\sin^2 \left(\frac{\pi k_x}{N} \right) + \sin^2 \left(\frac{\pi k_y}{N} \right) \right], \quad (5)$$

where N is the length of one side of the squared lattice and k_x and k_y are two integers under the condition $0 \leq k_x, k_y \leq (N - 1)$.

In all numerical simulations a Runge-Kutta method of fifth order with a time step $\Delta t = 0.01$ was used. We compared our results to an independent code where a Verlet algorithm with $\Delta t = 0.005$ was used and observed no differences. In the studies of one-dimensional systems the simulation of an infinite system was replaced with a finite chain of such a length that the fastest phonons could not make a turn and come back to the finite volume of the NLE excitation during the simulation time. In two dimensions such a method would mean a squared waste of computing time and ban us on parallel computers. However, there is another way to avoid recurrence of phonons which are radiated from the NLE: to switch on a (reflectionless) friction outside a given volume such that the radiated phonons will be captured and eliminated. The condition of reflectionlessness implies a gradual increase of the friction with growing distance or, in other words, a large number of collisions between phonons and friction applied lattice sites. The friction is added to the right-hand side of (4) in the form $-\gamma_{\vec{R}} P_{\vec{R}}$. In the case of a full system we work with a friction-free volume of size 20×20 and an additional friction-applied boundary of thickness ten particle distances on each side. Thus the overall number of particles is $40 \times 40 = 1600$. The friction is linearly increased in the friction-applied walls from zero up to a maximum value of γ_0 at the boundary layer. At the boundaries periodic boundary conditions are applied.

To proceed we have to optimize the maximum friction coefficient, since for $\gamma_0 = 0$ or $\gamma_0 = \infty$ the phonons are completely transmitted or reflected, respectively. We simulate the linearized Φ^4 lattice $[V(z) = z^2, \Phi(z) = 1/2Cz^2]$ with an initial condition, where the central particle is displaced by $\Delta X = 1$ from its ground-state position, all other particles are held at their ground-state positions and the velocities are zero. The corresponding initial energy is $E = 1.1$. We let the system evolve and measure the energy stored in the system $E(t)$ and the energy stored in the central particle and its four neighbors $E_5(t)$ for $t = 2000$. The result is shown as a function of γ_0 in Fig. 1. We find that for the chosen geometry the optimum value for the maximum friction coefficient is $\gamma_0 \approx 0.005$. The full time dependence of the two energies $E(t)$ and $E_5(t)$ using $\gamma_0 = 0.005$ are shown in Fig. 2. We see that after waiting times of $t \leq 2000$ the central particle and its four neighbors lose more than 99.9% of their initial energy. In the following we will use the thus chosen value for the maximum friction coefficient $\gamma_0 = 0.005$ in all described simulations.

B. NLE solutions

Let us show a stable NLE solution. For that we prepare the following initial condition: a central particle at the ground-state position, nearest neighbors displaced to $X_{(nn)} = -1.01163$, the velocity of nearest neighbors $P_{(nn)} = 0.0225$, the velocity of the central particle is adjusted to the initial energy $E = 0.3$, and all other par-

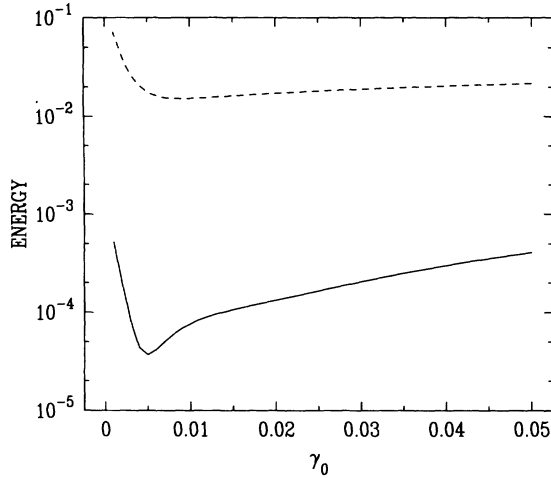


FIG. 1. Energy of the linearized Φ^4 lattice after waiting time $t = 2000$ as a function of γ_0 (cf. text). Dashed line, total energy E of the system; solid line, energy E_5 stored in the central particle and its four neighbors.

ticles are at their ground-state positions with zero velocities. To characterize the localization properties we use the local discrete energy density

$$e_{\vec{R}} = \frac{1}{2} P_{\vec{R}}^2 + V(X_{\vec{R}}) + \frac{1}{2} \sum_{\mathcal{N}} \Phi(X_{\vec{R}} - X_{\vec{R}'}) . \quad (6)$$

Let us define the energy stored on five particles [the central particle $\vec{R} = (0, 0)$ and its four neighbors]

$$e_5 = \sum_{\vec{R}'} e_{\vec{R}'}, \quad |\vec{R}'| \leq 1 . \quad (7)$$

In the inset in Fig. 3 we show e_5 as a function of time for the above given initial condition. Clearly we observe localization of vibrational energy for extremely long times. One has to keep in mind that the typical oscillation times are of the order of $t_0 = 4$. The stability property of

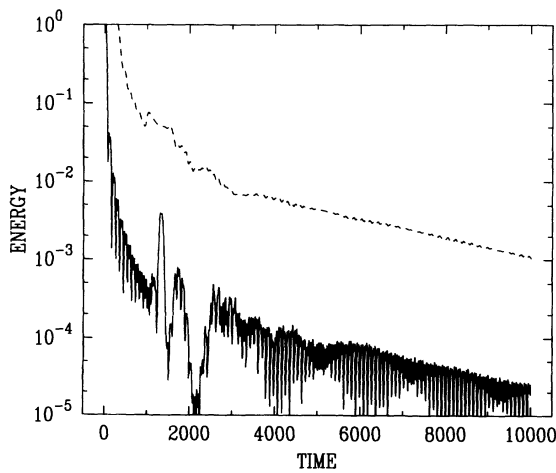


FIG. 2. Time dependence of the energy of the linearized Φ^4 lattice for $\gamma_0 = 0.005$. Dashed line, total energy E of the system; solid line, energy E_5 .

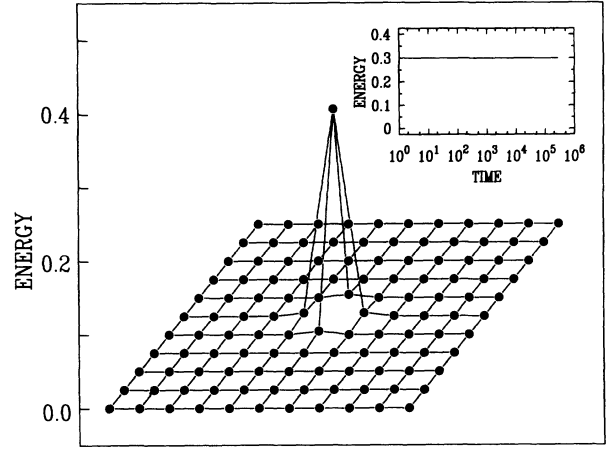


FIG. 3. Energy distribution for the NLE solution with initial energy $E = 0.3$ after waiting time $t = 3000$ (for initial conditions see text). The filled circles represent the energy values for each particle; the solid lines are guides to the eye. Inset: Time dependence of the NLE energy e_5 .

the observed NLE is very similar to examples from one-dimensional cases. The energy distribution in the NLE solution after $t = 3000$ is shown in Fig. 3. Essentially five particles are involved in the NLE motion: a central particle and its four nearest neighbors.

Since we used symmetrical initial conditions essentially two degrees of freedom are excited. To describe the NLE solution we construct a *reduced problem* in analogy to the one-dimensional problem. The reduced problem consists out of the five particles which are essentially involved in the NLE motion. The rest of the lattice is held at its ground-state position. Together with the consideration of symmetric initial conditions we are left with the following two degrees of freedom problem:

$$\ddot{Q} = Q - Q^3 + 4C(q - Q) , \quad (8)$$

$$\ddot{q} = q - q^3 + C(Q - q) - 3C(1 + q) . \quad (9)$$

Here $Q = X_{(0,0)}$ and $q = X_{(\pm 1, \pm 1)}$ are the coordinates of the central and nearest neighbor particles, respectively. In the one-dimensional case it was shown that certain solutions of the reduced problem correspond to NLE solutions in the full system [16, 17].

C. The reduced problem

Before we show that the same correspondence principle works for the two-dimensional example in the present work, we want to characterize the main features of the system of equations (8) and (9).

In Figs. 4(a)–4(d) we show Poincaré mappings for the reduced problem for energies $E = 0.2, 0.5, 2.5, 5$, respectively. As can be seen there the reduced problem is not integrable since we find stochastic motion. Thus the energy is the only integral of motion. However, we find islands of regular motion (regular islands) which are separated from each other by stochastic layers. The topology of the stochastic layers indicates the topology of de-

stroyed separatrices. For small energies $E = 0.2$ [Fig. 4(a)] the thickness of the stochastic layer is too small to be detected at all (in the presented resolution) so that we find two regular islands which we label with the numbers 1 and 2. The elliptic fixed points of each regular island correspond to time-periodic solutions of the reduced problem. Increasing the energy we find a rather abrupt increase of the thickness of the stochastic layer for $0.35 < E < 0.4$. Thus at $E = 0.5$ [Fig. 4(b)] we are faced with effects of period doubling (increasing number of regular islands) and a decrease of the size of the islands. For $E = 2.5$ [Fig. 4(c)] nearly the whole available phase space is filled with chaotic trajectories. However, for higher energies [here $E = 5$ in Fig. 4(d)] the size of the regular islands increases again. In the limit $E \rightarrow \infty$ the reduced problem becomes infinitely close to an integrable system of two noninteracting quartic oscillators.

A proper characterization of the regular islands is the frequency of their corresponding elliptic fixed points. In Fig. 5 the fixed point frequencies of the main regular islands are shown as a function of energy. For small energies the frequencies of the fixed points of regular islands 1 and 2 become the eigenfrequencies of the linearized problem (around the groundstate): $\omega^2 = 2 + 2C$ for island 1

and $\omega^2 = 2 + 6C$ for island 2, both of the frequencies are in the phonon band of the infinite system (5). From Fig. 5 it follows that there is a nonzero lower energy threshold above which the fixed point frequency from island 1 becomes nonresonant with the phonon band.

For reasons discussed below we concentrate on island 1. We denote its fixed point frequency by ω_1 (here the index refers not to the island number but to the degree of freedom excited in the island). Then several statements can be made with respect to the secondary degrees of freedom which can be excited (cf. the torus intersection structure around the fixed point in island 1). Considering an infinitesimally small excitation of the second (symmetric) degree characterized by its frequency ω_2 one can show that in the limit of zero energy $\omega_2^2 = 2 + 6C$ (cf. the Appendix). If one lifts the symmetry of the initial conditions in the reduced problem one has to consider the generalized reduced problem

$$\ddot{Q} = Q - Q^3 + \sum_{i=1}^4 C(q_i - Q) , \quad (10)$$

$$\ddot{q}_i = q_i - q_i^3 - 3C(1 + q_i) + C(Q - q_i) . \quad (11)$$

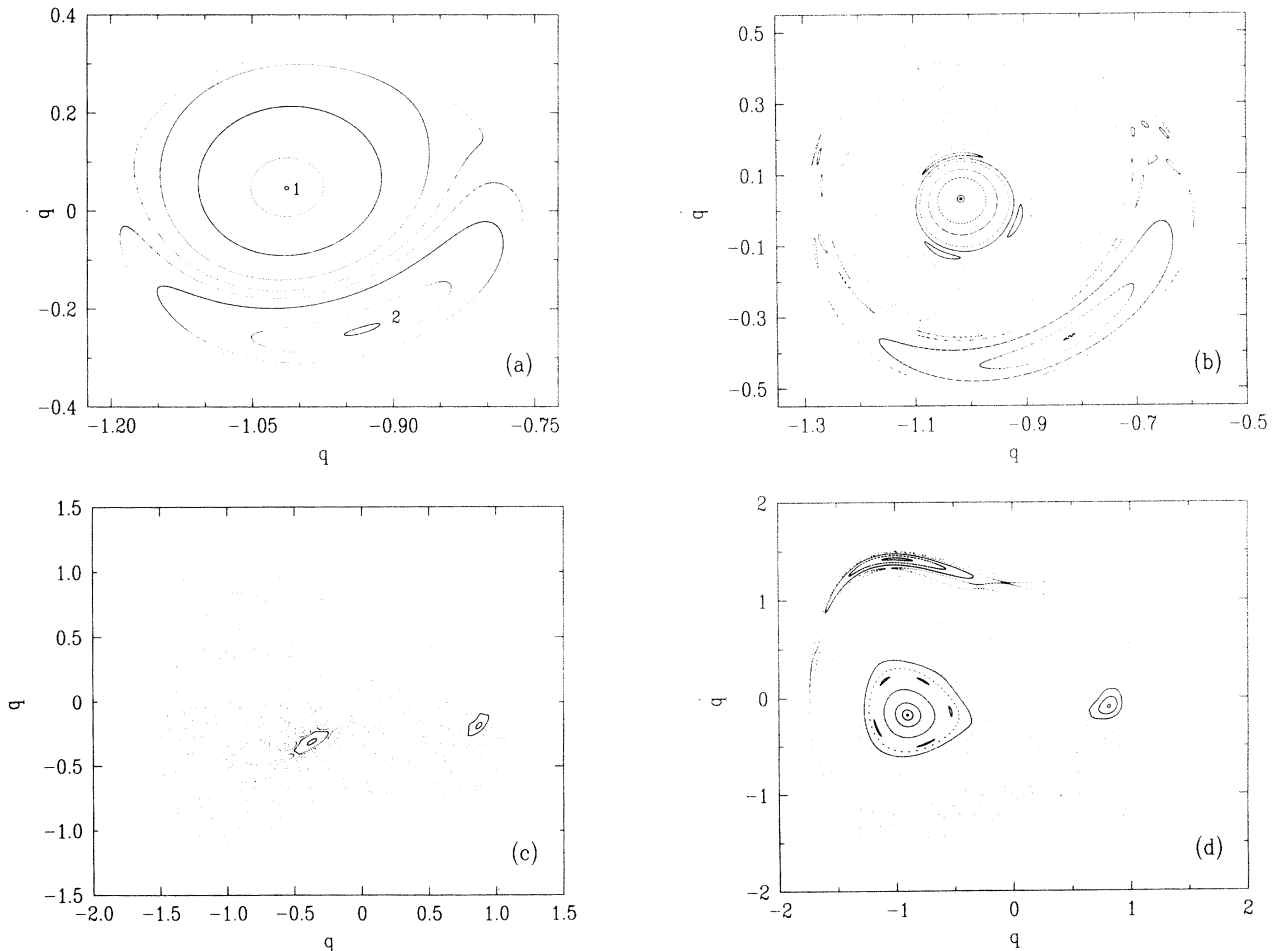


FIG. 4. Poincaré intersection between the trajectory of the symmetric reduced problem and the subspace $\{\dot{q}, q, Q = -1, \dot{Q} > 0\}$. (a) $E=0.2$; (b) $E=0.5$; (c) $E=2.5$; (d) $E=5.0$.

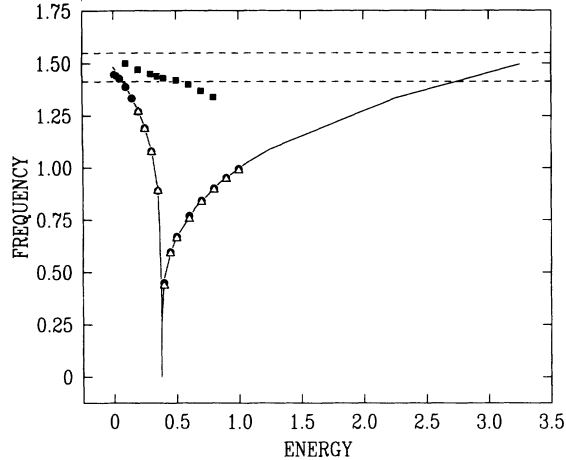


FIG. 5. Energy dependence of the frequency. Filled circles, fixed point frequency from regular island 1 in Fig. 4(a); filled squares, fixed point frequency from regular island 2 in Fig. 4(a); open triangles, frequency ω_1 of the periodic NLE solution from the full system; solid line, frequency of the effective potential; dashed lines, positions of the phonon band edges.

Here $Q = X_{(0,0)}$ as in (8) and (9) and the four coordinates q_i , $i = 1, 2, 3, 4$, denote the coordinates of the four nearest neighbors of the central particle. Since we deal with five degrees of freedom now we have to expect five (instead of two) fundamental frequencies. The system (10) and (11) has rotational symmetry of order 4. It follows (cf. the Appendix) that the three new frequencies $\omega_3, \omega_4, \omega_5$ are equivalent to each other in the limit of infinitely small asymmetric perturbations of the fixed point periodic solution. In the limit of zero energy it follows that $\omega_3^2 = \omega_4^2 = \omega_5^2 = 2 + 4C$. Increasing the energy from its lowest value leads to a decrease of all five frequencies. The inequality $\omega_1 < \omega_{3,4,5} < \omega_2$ (which is true only for low energy values) determines the sequence of the ω_i crossings of the lower phonon band edge.

D. The correspondence principle

Let us show the connection between the reduced problem and the NLE solutions of the full system. For that we plot in Fig. 5 the frequencies of (nearly) periodic NLEs as a function of energy. We observe very good agreement with the data of the fixed point frequency ω_1 from island 1 of the reduced problem. In fact one can check that the whole time-dependent periodic NLE solution of the full system is very close to the corresponding fixed point periodic solution from island 1 of the reduced problem. Since the frequency ω_2 of the symmetric perturbation of the fixed point periodic NLE solution according to the results from the reduced problem is in resonance with phonon frequencies up to energy values of 1, we increase the energy to $E = 5$ [cf. Fig. 4(d)] and perform a Poincaré mapping for the NLE solutions of the *full system*. The result is shown in Fig. 6 together with the corresponding data from the reduced problem [cf. Fig. 4(d)]. The result is amazing: the torus intersections are

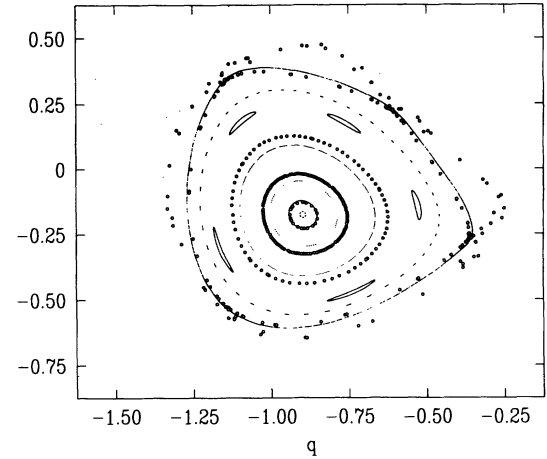


FIG. 6. Poincaré intersection as in Fig. 4(d), except for the following: open circles, result for the full system; dots, result for the symmetric reduced problem [taken over from Fig. 4(d)]. Note that because of the high density of dots solid lines can be formed.

practically identically for the two-frequency NLE solution from the full system and the corresponding regular trajectories from the regular island of the reduced problem. If one chooses an initial condition in the full system that corresponds to the chaotic trajectory in the reduced problem [Fig. 4(b)], then we find a quick decay of the energy excitation in the full system as shown in Fig. 7.

If the energy is low enough the frequency ω_2 of the symmetric perturbation of the periodic NLE will come into the phonon band. Then we expect a loss of the energy part stored in the corresponding second degree of freedom, leaving the main degree of freedom essentially unaffected. To show that we simply perform a Poincaré mapping for the case mentioned. The result is shown in Fig. 8. Indeed instead of an intersection line with a torus we find a spiral-like relaxation of the NLE solution onto the periodic fixed point NLE. The fixed point periodic

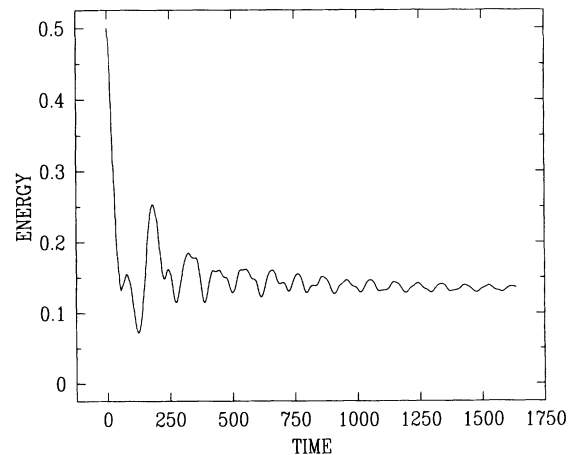


FIG. 7. Time dependence of the NLE energy in the full system for initial condition corresponding to chaotic trajectory in Fig. 4(b).

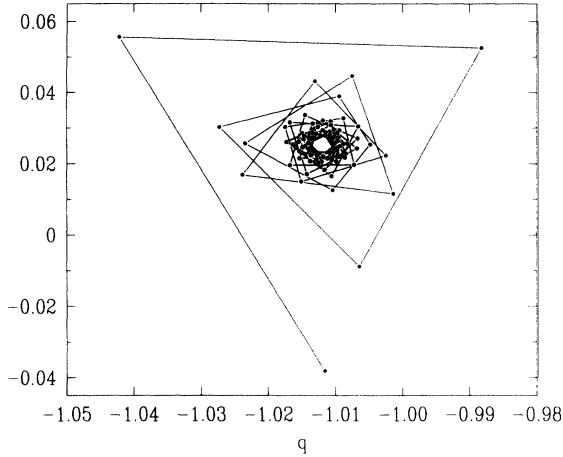


FIG. 8. Poincaré intersection (as in Fig. 4) but for the full system with initial condition $X_{|\vec{R}|=1} = -1.0116$, $\dot{X}_{|\vec{R}|=1} = -0.038112$, and all other particles are at ground-state position and zero velocity, except the velocity of particle $\vec{R} = 0$ (adjusted to energy $E = 0.3$). The filled circles are the actual mapping results. The lines are guides to the eye and connect the circles in the order of their appearance. The spiral-like form of the broken line indicates the evolution of the contraction of the NLE solution to the fixed point periodic NLE solution.

NLE acts like a limit circle, although the whole system is conservative.

E. Effective potential

Because of the smallness of the nearest neighbors amplitudes compared to the amplitude of the central particle in a NLE solution, we can try to account approximately for the motion of the central particle assuming that the nearest neighbors are at rest at their ground-state positions. Then the central particle would move in an effective potential

$$V_{\text{eff}}(z) = V(z) + 2C(z+1)^2. \quad (12)$$

The motion in this potential is periodic with an energy-dependent (or amplitude-dependent) period $T_1 = 2\pi/\omega_1$. Since most of the energy in the NLE solution is concentrated on the central particle and its binding energy to the nearest neighbors, it is reasonable to compare the results for the energy dependence of ω_1 for (12) with the numerical result as given in Fig. 5. As can be seen in Fig. 5, the overlap between the result from the effective potential, the reduced problem, and the full system are very good. Thus we have a proper method for predicting the behavior of the main NLE frequency ω_1 as a function of energy. This method is directly taken over from the known results in the one-dimensional case.

F. Stability properties

As it was shown in [15, 16] for the one-dimensional case, it is possible to carry out a stability analysis for pe-

riodic NLEs (i.e., the fixed point solutions) with respect to extended phononlike perturbations. In fact the procedure for the stability analysis in the two-dimensional case is exactly the same. Thus we will highlight here only the necessary parts of the steps one has to follow. We assume that we know an exact periodic NLE solution $X_{\vec{R}}(t)$. Then we consider a slightly perturbed trajectory $\tilde{X}_{\vec{R}} = X_{\vec{R}}(t) + \Delta_{\vec{R}}(t)$. Since the assumed NLE solution is localized, it becomes infinitely small for large distances from the NLE center. This circumstance does not pose a serious problem for the definition of the expression “slightly perturbed.” One can just consider small amplitude oscillations (phonons) around the ground state of our system. Then we have a well defined small parameter determining the weak nonlinear corrections to the linear equations. We take over this definition of smallness to our problem. In the center of the NLE the perturbation will thus be small compared to the NLE contribution. Far away from the center the perturbation can even become large compared to the NLE contribution, but it will be still small enough to ensure the linearized equations work well. Then we can consider small perturbations of the NLE solution which are extended.

In the next step we insert the perturbed ansatz into the lattice equations of motion. Using the fact that the unperturbed part is a solution of the equations of motion and linearizing the equations with respect to the perturbation yields a set of coupled differential equations with time-dependent (periodic) coefficients. In analogy to [16] we can define a map, the stability of which is equivalent to the nongrowing of the small perturbation of the NLE solution. The sufficient condition for the stability is that neither of any multiple of half the NLE frequency is equal to a phonon frequency (5):

$$\frac{\omega_{k_x, k_y}}{\omega_1} \neq \frac{n}{2}, \quad n = 0, 1, 2, \dots \quad (13)$$

As we see this result explains the existence of an energy threshold (gap in the density of NLE states) for the NLE solutions. Because the NLE frequencies according to the reduced problem will always lie in the phonon band for small enough NLE energies, the low energy NLEs are unstable against smallest perturbations. In the one-dimensional case this statement was tested in the full system using an entropy-like variable measuring the degree of energy localization [16]. On approaching the energy threshold (predicted by the results of the reduced problem together with the stability analysis) from above the entropy drastically increases at the predicted threshold value. It is still possible that low energy NLEs exist with a very small degree of localization and with frequencies very close to the phonon band edge, but outside the band itself. In the two-dimensional case considered here we also observe a very sharp transition in the degree of localization at the predicted energy threshold value. In fact it becomes impossible to find a NLE solution with energies below the threshold value. That indicates the tiny phase space part at low energies which still might be occupied with weakly localized states.

A more subtle problem is the *internal* stability of periodic NLEs. As it is known for several one-dimensional

systems, periodic NLE solutions can become internally unstable, i.e., a weak symmetry breaking perturbation of the periodic NLE will transform the NLE solution into other existing periodic NLEs of different parity or even into NLEs moving through the lattice [9, 13, 26]. Currently it is unclear how to classify and find the different possible periodic NLE solutions on a two-dimensional lattice. Efforts to do so are reported in [21]. We wish to emphasize that the periodic NLE solutions reported in this paper are certainly not the only ones allowed to exist in the underlying lattice. Thus we can only make statements about the internal stability of the NLE solutions considered in the present work. Using the results of the linearization of the equations of motion around the periodic NLE solutions (see the Appendix) we can trace the values of the squared secondary eigenfrequencies $\omega_2^2, \omega_{3,4,5}^2$ and can report here that throughout the considered cases all squared eigenfrequencies are positive. Consequently the periodic NLE solutions discussed here are internally stable.

The results of the *stability* analysis drawn above do not allow us to conclude about the *existence* of NLE solutions in a strict general sense. As it was shown in [25] for the one-dimensional case, periodic NLEs do not exist if any multiple of the NLE frequency resonates with phonon frequencies [this condition corresponds to the cases of even integers n in (13)]. Also all multiple frequency NLEs are strictly speaking unstable, since it is always possible to find combinations of multiples of two or more frequencies (whose ratio is irrational) resonating with phonon frequencies. It appears currently unclear how to take over the methods used in [25] for the one-dimensional case and to the two-dimensional case in order to obtain the existence criteria for NLE solutions. However, it can be expected that the methodological problems do not alter the results obtained in the one-dimensional case.

As it was shown in [27] the decay of the periodic NLE solutions far away from the NLE center can be well described by a Green's function method, which yields exponential decay in the amplitudes.

IV. DISCUSSION

In the present work we have shown that it is possible to take over the results on the existence and properties of nonlinear localized excitations in nonlinear lattices from lattice dimension one to lattice dimension two. Thus several goals were achieved: (i) the existence of NLEs in two-dimensional lattices is verified, (ii) the theory developed for NLEs in one-dimensional systems appears to be of validity independent on the lattice dimension, and (iii) the power of the theoretical framework to predict the existence of NLE solutions in several one-dimensional lattices has been extended by its correct prediction of the NLE existence in higher-dimensional lattices. Thus the NLE existence in three-dimensional lattices can be considered as highly likely. There is at the present no single reason supporting the nonexistence of NLEs due to lattice dimensions.

Besides the analysis of the properties of the secondary frequencies (cf. the Appendix) the present work has also

shown that the resonating of secondary frequencies with phonon frequencies does not imply a shrinkage of the phase space part of the system corresponding to NLE solutions. Indeed as long as the main frequency ω_1 stays outside the band, the choice of an initial condition with excited secondary degrees of freedom will still yield a NLE. If the secondary frequencies are outside the phonon band as well, the solution will be a (very weakly) decaying multiple frequency NLE. If the secondary frequencies resonate with the phonon band, the corresponding energy part stored in the NLE is radiated away and the NLE "collapses" onto its periodic fixed point solution. This attractorlike behavior ensures that there is still a finite phase space volume around the fixed point periodic solution which corresponds to NLEs even after extremely long waiting times. Thus we have strong evidence for the statistical relevance of NLE solutions in corresponding lattices at finite temperatures. Indeed the only case when NLEs can become statistically unimportant is when the main frequency ω_1 resonates with the phonon band.

We can conclude from our results on the energy radiation of perturbed periodic NLEs and from the mentioned existence proofs for periodic NLEs that the results on radiation processes accounted for in [28] are wrong. In order to get the leading order radiation of perturbed periodic NLEs one has to linearize the phase space flow of the system around the unperturbed periodic NLE solution and *not* around the ground state of the system as it was done in [28].

Let us finally address the following question: What are the physical applications where one can expect NLEs to exist? In the mathematical sense the answer is when the main frequency ω_1 can be "pulled out" of the phonon band with increasing energy. To check the behavior of the main frequency we have to construct the effective potential. Consider, e.g., a monoatomic crystal. The pair potential of interaction is usually an asymmetric potential around the stability position. The effective potential can be constructed exactly as described in Sec. III. If the repelling part of the pair potential goes nonlinearly enough, then there can be oscillations of a particle in the effective potential with frequencies above the phonon band. However, one has also to check the minimum energy (energy threshold) required for the NLE existence. As studies for a particular class of crystals have shown, NLEs cannot be excited there thermally because the melting point is too low. However, it could still be possible to excite the NLEs locally nonthermally [29]. If we consider crystals with many atoms per unit cell, we can expect at least the existence of phonon gaps between acoustic and different optical zones. It is a well known approach to describe structural phase transitions with the use of Φ^4 -like models, simulating the behavior of certain soft phonon modes essentially decoupled from other nonsoftening modes [30]. However, there might be too many problems on this path to really make sure that Φ^4 -lattice-type NLEs can exist in such crystals. Another way of thinking leads us to the fact that the adding of a periodic external field (onsite potentials) can produce a finite phonon gap eliminating the conservation of mechanical momentum. Such situations are very likely in the case of atomic monolayers on proper

substrate surfaces. If it becomes possible to choose such cases, where the phonon band width becomes small compared to the gap width, NLEs could exist. With these arguments we did not intend to judge the different physical situations where NLEs are likely or unlikely to exist. It was the search strategy we had in mind. It is one of the forthcoming tasks to provide a foundation for these ideas in order to proceed in the question of applicability. Still the mathematical result that NLEs are generic solutions of nonlinear lattices [19] serves as a powerful indicator of their relevance in different physical realizations.

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APPENDIX

Here we consider Eqs. (10) and (11) (the reduced problem describing NLE solutions). We consider a periodic NLE solution at a certain energy E : $Q^{(p)}(t + 2\pi/\omega_1) = Q(t)$, $q_j^{(p)}(t + 2\pi/\omega_1) = q_j(t)$. This solution represents a closed orbit in the phase space of the reduced problem. If the system is integrable in a neighborhood of the closed orbit, then each phase space trajectory from this neighborhood belongs to some surface, which is diffeomorphic to a five-dimensional torus [31]. Then we can introduce some new set of canonically conjugated coordinates Π_n, Q_n , $i = 1, 2, 3, 4, 5$ such that

$$Q_n = J_n \sin \omega_n t, \quad \Pi_n = \omega_n J_n \cos \omega_n t. \quad (\text{A1})$$

Here $J_n, \Theta_n = \omega_n t$ denote the action-angle variables. Without loss of generality we define the mentioned periodic orbit with

$$\mathbf{M} = \begin{pmatrix} 4C - 1 + \alpha & -C & -C & -C & -C & -C \\ -C & 4C - 1 + \beta & 0 & 0 & 0 & 0 \\ -C & 0 & 4C - 1 + \beta & 0 & 0 & 0 \\ -C & 0 & 0 & 4C - 1 + \beta & 0 & 0 \\ -C & 0 & 0 & 0 & 4C - 1 + \beta & 0 \\ -C & 0 & 0 & 0 & 0 & 4C - 1 + \beta \end{pmatrix} \quad (\text{A6})$$

with

$$\alpha = 3|A_0^{(p)}|^2 + 6 \sum_{k=1,2,\dots} |A_k^{(p)}|^2, \quad (\text{A7})$$

$$\beta = 3|a_0^{(p)}|^2 + 6 \sum_{k=1,2,\dots} |a_k^{(p)}|^2. \quad (\text{A8})$$

From (A7) and (A8) it follows that $\alpha = 3\langle Q^{(p)^2}(t) \rangle$ and $\beta = 3\langle q^{(p)^2}(t) \rangle$, where the symbol $\langle A(t) \rangle$ means the time average of the (periodic) function $A(t)$. Because of (A5) all squared frequencies ω_n^2 have to be equal to the eigen-

$$J_1 \neq 0, \quad J_n = 0 \quad (n = 2, 3, 4, 5). \quad (\text{A2})$$

For trajectories from a neighborhood of the periodic orbit the old displacements and momenta will be some functions of the new coordinates. These functions can be expanded in Taylor series in the new coordinates. In the limit $J_{2,3,4,5} \ll J_1$ the old coordinates will be a sum of the unperturbed periodic orbit solution and four perturbations each periodic with its own frequency $(\omega_{2,3,4,5})$. Then we can represent the perturbed solution in a Fourier series:

$$Q(t) = \sum_{k=0,\pm 1,\pm 2,\dots} A_k^{(p)} e^{ik\omega_1 t} + \sum_{n=2,3,4,5} (A_n e^{i\omega_n t} + A_n^* e^{-i\omega_n t}), \quad (\text{A3})$$

$$q_j(t) = \sum_{k=0,\pm 1,\pm 2,\dots} a_{j,k}^{(p)} e^{ik\omega_1 t} + \sum_{n=2,3,4,5} (a_{j,n} e^{i\omega_n t} + a_{j,n}^* e^{-i\omega_n t}). \quad (\text{A4})$$

In the limit $J_{2,3,4,5} \ll J_1$ it follows that $|A_n| \ll |A_k^{(p)}|$ and $|a_{j,n}| \ll |a_{j,k}^{(p)}|$. Because we deal with real functions $A_k^{(p)} = A_{-k}^{(p)*}$ and $a_{j,k} = a_{j,-k}^*$ have to be satisfied.

In the next step we insert (A3) and (A4) into the equations of motion of the reduced problem (10) and (11) and set equal to each other the terms on both sides of the five equations containing the exponential $e^{i\omega_n t}$. The result is a linear set of equations for the five (infinitely small) Fourier components $A_n, a_{j,n}$. If we set equal the terms containing the inverse exponential, the resulting algebraic equations are identical. Moreover since the resulting set is linear and all coefficients are real, it decomposes into two identical sets of equations for the real and imaginary parts of the Fourier components $A_n, a_{j,n}$. The resulting algebraic problem is an eigenvalue problem:

$$\omega_n^2 \vec{r} = \mathbf{M} \vec{r}. \quad (\text{A5})$$

Here the vector \vec{r} has five components and the matrix \mathbf{M} is given by

values of the matrix \mathbf{M} in (A6). Since the matrix \mathbf{M} has five eigenvalues, and the number of considered frequencies was four, there is one eigenvalue left. This eigenvalue is nothing else but the squared frequency ω_1^2 of the periodic orbit itself. Indeed a small perturbation of the given periodic orbit can be such that a new periodic orbit at a slightly changed energy is created (because the considered periodic orbits form a one-parameter family of solutions, where the parameter is the frequency ω_1 or the energy of the solution). Since we exclude cases when the periodic orbit is located on a separatrix, the change

of the frequency ω_1 under the considered perturbation is a smooth function of the perturbation. Thus in first order of the perturbation (which is considered here) the change of the frequency ω_1 does not show up (it will show up in second order of the perturbation).

The eigenvalue problem (A5) and (A6) has rotational symmetry of order 4 (this corresponds to the fact that the periodic NLE orbit is a symmetric solution on the squared lattice). Then there exists a linear operator g acting on the five-dimensional space spanned by the eigenvectors ξ_n of M such that

$$g\xi_n = \xi_{n'} \quad , \quad g^4\xi_n = \xi_n \quad . \quad (A9)$$

It follows that there can be no more than four asymmetric eigenvectors $g\xi_n \neq \xi_n$. But since their sum is invariant under g , it follows that they span a three-dimensional subspace (cf. Appendix 10 in [31]). Thus we end up with three asymmetric eigenvectors of (A6) with threefold degenerated eigenvalues

$$\omega_3^2 = \omega_4^2 = \omega_5^2 = 4C - 1 + \beta \quad . \quad (A10)$$

The remaining two symmetric eigenvectors of (A6) are nondegenerated. They can be calculated by constructing the 2×2 matrix of all symmetric perturbations of the periodic orbit in analogy to the general case treated above. The resulting frequencies are given by

$$\omega_{\pm}^2 = \frac{1}{2}[\alpha + \beta \pm \sqrt{(\alpha - \beta)^2 + 16C^2}] + 4C - 1, \quad (A11)$$

$$\omega_1 = \omega_- \quad , \quad \omega_2 = \omega_+ \quad .$$

Result (A11) cannot be considered as a definition of ω_1 because one actually has to know α and β , which are functions of ω_1 .

In the limit of low energies (small amplitudes of oscillations) of the reduced problem it follows that $\alpha = \beta = 3$ and the frequencies will all lie inside the phonon band of the extended lattice:

$$\omega_1^2 = 2 + 2C \quad , \quad \omega_2^2 = 2 + 6C \quad , \quad \omega_{3,4,5}^2 = 2 + 4C \quad . \quad (A12)$$

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