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Existence of localized excitations in nonlinear Hamiltonian lattices

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We consider time-periodic nonlinear localized excitations (NLE's) on one-dimensional translationally invariant Hamiltonian lattices with an arbitrary finite interaction range and an arbitrary finite number of degrees of freedom per unit cell. We analyze a mapping of the Fourier coefficients of the NLE solution. NLE's correspond to homoclinic points in the phase space of this map. Using dimensionality properties of separatrix manifolds of mapping we show the persistence of NLE solutions under perturbations of the system, provided that the NLE's exist for the given system. For a class of nonintegrable Fermi-Pasta-Ulam chains, we rigorously prove the existence of NLE solutions.

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I. INTRODUCTION

The existence, stability, and properties of nonlinear localized excitations (NLE's) in Hamiltonian lattices with discrete translational symmetry have been subjects of growing research interest (see, e.g., [1–4] and references therein). NLE's can be viewed as generalized discrete analogs to the breather solution in a sine-Gordon equation [2]. They are characterized by a localized vibrational state of the lattice. There are two basic reasons for the generic NLE existence on Hamiltonian lattices: (i) the lattice forces acting on a given particle are *nonlinear* (thus one can tune oscillation frequencies by varying the energy) and (ii) the *discrete translational symmetry* of the lattice (in contrast to the continuous translational symmetry of Hamiltonian field equations) provides a *finite* upper phonon band edge of the spectrum of extended small amplitude oscillations of the lattice around its ground state [5,6].

There are a few known rigorous NLE existence proofs. First NLE's are exact solutions of the *integrable* Ablowitz-Ladik lattice [7]. In fact, they form a three-parameter family of solutions. Second, NLE's are exact solutions for the Fermi-Pasta-Ulam chain with a boxlike interaction potential [8]. In this case, the NLE's are of compact support. Finally, and most importantly, MacKay and Aubry have derived an existence proof for NLE's in an array of weakly coupled anharmonic oscillators [9]. Remarkably, this existence proof works independent of the lattice dimension.

In this contribution, we will first deal with the existence of NLE's in *nonintegrable* generic one-dimensional Hamiltonian lattices. In the second part, we will investigate a class of Fermi-Pasta-Ulam chains and give rigorous proofs for the NLE existence.

Let us briefly outline the main steps in the approach presented below. We will assume the existence of a time-periodic NLE on a one-dimensional lattice. We represent the lattice displacements at each lattice site in the NLE ansatz in a Fourier series with respect to time. When we insert the NLE ansatz into the lattice equations of motion, we obtain a set of coupled algebraic equations for the Fourier components of the NLE ansatz, which form an infinite-dimensional map. The NLE solution has to correspond to a common point of two separatrix manifolds in the phase space of the map, or a homoclinic point. Analyzing the map in the (linearizable) tails of the NLE, we can derive the dimension of the separatrix manifolds. Consequently, we show that if a homoclinic point exists for a given system, then generically the homoclinic point will survive under perturbations of the system. We then consider a subclass of Hamiltonian chains and rigorously prove the existence of two different (with respect to symmetry) NLE solutions. For this particular example, we show the emergence of horseshoe patterns—a consequence of the existence of homoclinic points.

II. STABILITY OF NLE SOLUTIONS UNDER HAMILTONIAN PERTURBATIONS

We consider a classical one-dimensional Hamiltonian lattice of interacting particles (perhaps feeling an external field periodic with the lattice) with lattice cite $a = 1$. The displacements of the particles from their ground state (equilibrium) positions are given by a n-dimensional vector $\vec{X}_l$, where n is the number of components per unit cell ($n \leq n_0$, n_0 finite) and the integer l marks the number of the unit cell. The range of the interaction r is considered to be finite: $r \leq r_0$, r_0 finite. Here, n_0 and r_0 are positive integers. The potential energy of the system is required to have anharmonic terms in the displacements if expanded in a Taylor series around the ground state (minimum of potential energy) of the system. Furthermore, the potential energy should become a positive definite quadratic form in the limit of infinitely small displacements. The Hamilton function H is given by the sum of the kinetic energy of all particles and the potential energy.

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As it was shown in [5],[6], the only possible *exact* NLE solution on an arbitrary lattice (by that we mean no additional symmetries are present) has to have the form,

$$\vec{X}_l(t) = \vec{X}_l(t + 2\pi/\omega_1) \ , \ \vec{X}_{l\to\pm\infty} \to \vec{0} \ . \qquad (1)$$

Then one can avoid resonance conditions of multiples of the fundamental frequency ω_1 [as they appear in the Fourier transformed functions in (1) with respect to time, because of the nonlinearity of the system], with phonon frequencies of the linearized (around the groundstate) system. Since the motion of assumed existent NLE's requires the excitation of at least a second fundamental frequency in the ansatz (1) [10], we can exclude them from the consideration and search for stationary time-periodic NLE's as given in (1). Note that in the case of the Ablowitz-Ladik lattice, additional symmetries are present (the lattice is integrable) and, thus, the above statement does not hold—moving NLE's are exact solutions in this nongeneric case.

Because of the assumed time periodicity of all displacements in (1) we obtain, for the assumed NLE solution,

$$\vec{X}_l = \sum_{k=0,\pm1,\pm2,\ldots} \vec{A}_{(l,k)} e^{i\omega_1 kt} \ . \qquad (2)$$

Now we can insert this ansatz (2) into the Newtonian equations of motion $\ddot{\vec{X}}_l = \partial H/\partial \vec{X}_l$. The left and right hand expressions of the equation of motion are represented again as a general Fourier series. Equaling the prefactors at identical exponential terms to each other, we finally obtain a coupled set of algebraic equations for the unknown Fourier coefficients $\vec{A}_{(l,k)}$. Because of (1), the Fourier coefficients have to satisfy the boundary condition $\vec{A}_{(l\to\pm\infty,k)} \to 0$. In the following, we will study properties of this algebraic set of equations.

First we can note that, because of the $d = 1$ dimensionality of the considered lattice, the coupled set of algebraic equations for the Fourier coefficients $\vec{A}_{(l,k)}$ can be represented as a discrete map of a $d_M = (2r_0 n_0 k_{\max})$-dimensional phase space, where the integer $k_{\max}$ represents the number of considered higher harmonics in (2) and has to tend to infinity. In other words, given the Fourier coefficients at $2r_0$ neighboring lattice sites completely determines the Fourier coefficients to the left and right of the specified chain segment. Second, because of the required asymptotic vanishing of the Fourier coefficients for $l \to \pm\infty$, we can linearize the d_M-dimensional map in the tails of the assumed NLE solution with respect to the variables $\vec{A}_{(l,k)}$. The linearized map will decouple into a set of $k_{\max}$ independent $d_s = 2r_0 n_0$-dimensional linear submaps [6]. In each of these submaps, Fourier components with only one Fourier integer k will appear. Each linear submap is equivalent to the problem of finding solutions of the linearized (around the ground state) lattice equations of motion using the ansatz $\vec{X}_l(t) = A_l \exp(i\tilde{\omega}t)$. Here, for every submap, one has to substitute $\tilde{\omega} = k\omega_1$. If $\tilde{\omega}$ equals an arbitrary phonon frequency of the linearized lattice equations, then it follows that the corresponding linear submap is characterized by a matrix $\mathbf{M}_k$ of dimension $d_s \times d_s$ with $\det\mathbf{M}_k = 1$ and $\lambda_i\lambda_{i+d_s} = 1$, where $\lambda_{i,i+d_s}$ are two of the $2d_s$ eigenvalues of $\mathbf{M}_k$. Since these properties do not depend on the specific value of the considered phonon frequency, it follows that they are independent of $\tilde{\omega}$ and thus independent of k and ω_1. Consequently, we find that every linear submap is volume preserving and symplectic.

Finally, we note that for every considered linear submap (and thus, also, for the original d_M-dimensional map), the phase space point of zero Fourier components is a fixed point on the map. If $k\omega_1$ equals a phonon frequency, the fixed point is of elliptic character. If, however, $k\omega_1$ does not equal any phonon frequency, the fixed point has to be a saddle point (because it can not be an elliptic fixed point and the map is symplectic). That means that $r_0 n_0$ eigenvalues of the matrix $\mathbf{M}_k$ are real and of an absolute value lower than one. Consequently, the separatrix manifold of all points in the space of the submap attracted by the saddle point is of dimension $d_{\rm SM} = r_0 n_0$.

If we require that neither of the multiples of the fundamental frequency $k\omega_1$ resonates with the phonon band, the corresponding original d_M-dimensional map in the phase space of the Fourier coefficients has a separatrix manifold of dimension $d_M/2$. To get a NLE solution, we have to find a point in the space of the original map which belongs simultaneously to the separatrix manifold S_- attracting the solution to zero for $l \to -\infty$ and to the separatrix manifold S_+ attracting the solution to zero for $l \to +\infty$ (cf., e.g., [11,12]). This point has to be a homoclinic point then [13]. If a homoclinic point exists, there exist an infinite number of homoclinic points, which can be obtained by subsequent mapping of a given homoclinic point. As a result the horseshoe structure of intersections between the stable and unstable manifolds have to emerge [13].

Because of the assumed nonresonance condition (see above), every manifold has dimension $d_M/2$. Let us choose one of the homoclinic points. Then we can define the tangent planes to each of the two manifolds in this point. There are two possibilities for the topology of these two planes. Either (i) these two planes span the whole phase space of the map (of dimension d_M) or (ii) the two planes span a space of lower dimension than d_M. In case (i), any small perturbation of the original system (consequently of the map, consequently of the two manifolds, and consequently of the two tangent planes) will only shift the homoclinic point smoothly. Also in this case (i) all other homoclinic points will have the same topology with respect to the tangent planes. In case (ii) there exist perturbations of the system which will lead to a vanishing of the homoclinic point (and thus of all other homoclinic points too). Still, there will exist a perturbation for case (ii) such that the homoclinic point is smoothly shifted *and* simultaneously the two tangent maps will span the whole phase space of dimension d_M.

Consequently we can conclude, that if we have a NLE solution which corresponds to a set of homoclinic points of type (i), then any small perturbation of the system will smoothly transform the NLE solution into a NLE solution. If we have a NLE solution, which corresponds to a set of homoclinic points of type (ii), we can always find a perturbation such that we transform the NLE solution into a NLE solution, which corresponds to a set of homoclinic points of type (i) and is then stable under subsequent small perturbations. From the above said it follows that NLE solutions, if they appear, are generically not isolated objects in the sense that small perturbations of the system either do not destroy them at all, or that a proper perturbation of the system will transform them into nonisolated solutions.

We have operated with finite phase space dimensions d_M. Of course d_M was not bounded from above, so that the limit $d_M \to \infty$ can be considered without altering the arguments.

Let us summarize the results obtained so far. If we assume that for a given Hamiltonian chain a NLE solution exists, then it corresponds to an infinite number of homoclinic points in the map as introduced above. If neither of the multiples of the frequency of the NLE solution resonate with the phonon band (nonresonance condition), then the dimension of the stable and unstable manifolds is exactly one half of the map's phase space. From topological arguments it follows then, that either the NLE solution is structurally stable — i.e., it is smoothly transformed under *any* perturbation of the Hamiltonian of the system, or there exists at least one perturbation of the Hamiltonian such, that the NLE solution is smoothly transformed into a structural stable one. Of course a perturbation of the Hamiltonian has to preserve the general structure of the map, i.e., we are not allowed to consider e.g., a two-dimensional perturbation, which would lead to the impossibility of defining the map.

A central point in the consideration so far has been the nonresonance condition. If this condition is violated for n values of $k\omega_1$, then the dimension of the stable and unstable manifolds is lowered by $(2n)$ to $(d_M - 2n)$. If an NLE solution exists for such a case, then the tangent planes of the two manifolds in a given homoclinic point cannot span the whole phase space of the map. Consequently, there will always be perturbations of the Hamiltonian such that the NLE solution will vanish. At this point it also becomes clear that in the analogous problem of a Hamiltonian field equation, where resonances can never be avoided [12], systems which allow for NLE solutions become isolated (see also [11]).

If a system is given with a NLE solution which fulfills the nonresonance condition, it could be possible that a given perturbation of the Hamiltonian would lead to a violation of the nonresonance condition. Consequently, one has to check in a given case, whether the nonresonance condition survives under a perturbation.

III. PROOF OF EXISTENCE OF NLE SOLUTIONS FOR FERMI-PASTA-ULAM CHAINS

In the second part of this work, we will prove rigorously the existence of NLE solutions for a class of Fermi-Pasta-Ulam chains governed by the following equations of motion:

$$\ddot{X}_l = -(X_l - X_{l-1})^{2m-1} - (X_l - X_{l+1})^{2m-1} \qquad (3)$$

with $m = 2, 3, 4, \ldots$. As it was shown in [6, 14], we can consider a time-space separation ansatz $X_l(t) = A_l G(t)$. Inserting the separation ansatz into (3), we get a differential equation for $G(t)$: $\ddot{G}(t) = -\kappa G^{2m-1}(t)$ and a two-dimensional map for the amplitudes A_l,

$$\kappa A_l = (A_l - A_{l-1})^{2m-1} + (A_l - A_{l+1})^{2m-1} \, . \qquad (4)$$

Here, $\kappa > 0$ is required in order to get a bound oscillatory solution for $G(t)$. The phase space properties of map (4) are shown in Fig. 1 for the case $m = 2$ and $\kappa = 1$. Below we will refer to particular patterns observed in Fig. 1. We consider cases when $A_l/A_{l-1} < 0$ and introduce $f_l = |-1|^l A_l$ with

$$\kappa f_l = (f_l + f_{l-1})^{2m-1} + (f_l + f_{l+1})^{2m-1} \, . \qquad (5)$$

Equation (5) can be viewed as a two-dimensional map $\mathbf{M}$ of a vector $\vec{f_l} = (f_l, f_{l-1})$: $\vec{f}_{l+1} = \mathbf{M}\vec{f_l}$. The task is then to show the existence of at least one value of $\kappa > 0$ such that (5) yields $f_{|l|} \geq f_{|l'|} > 0$ for $|l| < |l'|$ and $f_{l\to\pm\infty} \to 0$.

First, we note that for any value of κ the map (5) has a fixed point $\vec{f}_{fp1} = (0,0)$. Adding weak harmonic nearest neighbor interactions to (3) and considering the limit of vanishing harmonic interactions yields that the fixed point $(0,0)$ is a saddle point with eigenvalues $\lambda_{1,fp1} = 0$ and $\lambda_{2,fp1} = \infty$. Consequently, we find that there exist two one-dimensional separatrix manifolds S_+ and S_- of the map (5). All points in the two-dimensional phase space of the map belonging to $S_\pm$ are attracted to the saddle point after an infinite number of iterations for $l \to \pm\infty$. Second, it follows that for $\kappa_{fp2} = 2^{2m} f^{2m-2}$ the point $\vec{f}_{fp2} = (f, f)$ is also a fixed point (see also Fig. 1). Linearizing the map around $\vec{f}_{fp2}$ yields the elliptic character of $\vec{f}_{fp2}$. The two eigenvalues of the linearized map $\lambda_{1,fp2}$ and $\lambda_{2,fp2}$ obey the relations $|\lambda_{1,fp2}| = |\lambda_{2,fp2}| = 1$ and are given by the expression $\lambda_{12,fp2} = \tilde{\kappa} - 1 \pm i[1 - (1-\tilde{\kappa})^2]^{1/2}$, with $\tilde{\kappa} = 2/(2m-1)$.

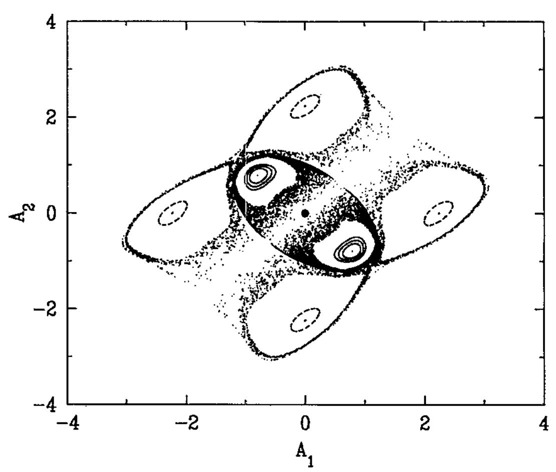

FIG. 1. Phase space of the map defined by (4) for $\kappa = 10$ and $m = 2$. The fixed points are $\vec{A}_{fp1} = (0,0)$ (solid circle), $\vec{A}_{fp2} = (\pm x, \mp x)$ ($x = 1/\sqrt{1.6}$, periodicity 2), $\vec{A}_{fp3} = (0, \pm y)$, and $(\pm y, 0)$ ($y = \sqrt{5}$, periodicity 4).

Let us mention another useful property of the map (5), which holds due to the discrete translational symmetry of the considered system (3). If we generate a sequence of $f_2, f_3, \ldots$ starting with a vector $\vec{f_1} = (a, b)$ and iterating (5) towards growing integers l, then we can generate the same sequence of numbers by iterating (5) towards decreasing integers l starting with the vector $\vec{f_1} = (b, a)$.

We consider an initial vector $\vec{f_l} = (a, b)$ with $0 < a \leq b$ and iterate towards increasing l. If we require $0 \leq f_{l+1} \leq a$, the parameter κ is confined to $\kappa_l^- \leq \kappa \leq \kappa_l^+$ with $\kappa_l^- = [(f_l + f_{l-1})^{2m-1} + f_l^{2m-1}]/f_l$ and $\kappa_l^+ = \kappa_l^- + (2^{2m-1} - 1)f_l^{2m-2}$. For any of the obtained values of $f_{l+1} = c$, we can consider the next step requiring $0 \leq f_{l+2} \leq c$. By itself, this requirement again yields a confinement of κ to $\kappa_{l+1}^- \leq \kappa \leq \kappa_{l+1}^+$. If we choose $c = 0$, then $\kappa_{l+1}^- = +\infty$. If we choose $c = a$, it follows $\kappa_{l+1}^+ \leq \kappa_l^+$. Because c is a monotonic function of κ, we can satisfy $a \geq f_{l+1} \geq f_{l+2} \geq 0$ only if $\kappa_l^- < \kappa \leq \kappa_l^+$ for $a = b$ and $\kappa_l^- < \kappa < \kappa_l^+$ for $a < b$. Repeating this procedure for every following lattice site, we get a sequence of monotonically increasing lower bounds on κ defined by the vanishing of $f_{l+m} = 0$ in the mth step. In the limit $m \to \infty$ we thus obtain exactly one value of κ, which is the limit of the mentioned sequence of lower bounds. This limiting value is finite, because it is always smaller than κ_l^+. It cannot be equal to κ_l^+ either, since we would then get the infinitely weak perturbed elliptic point of the map. Because of the elliptic character of this fixed point all amplitudes f_l have to stay infinitely close to their fixed point values which are finite. Thus we have found that for any initial vector $\vec{f_l} = (a, b)$ with $a \leq b$, there exists exactly one value of κ such that the initial vector belongs to S_+. The point $\vec{f_l} = (b, a)$ belongs then to S_-.

In the case $a = b$, it follows that it is always possible to find exactly one value of κ such that the initial vector $\vec{f_l} = (a, a)$ belongs to *both* S_+ and S_-. Consequently we proved rigorously the existence of one type of NLE's, which are known as "even-parity mode" [3]. Their characteristic feature is that the center of energy density of the corresponding solution is located between two lattice sites l and $(l - 1)$ at $(l - 0.5)$ [10].

Finally, let us consider the case $0 \leq f_{l-2} = f_l = a \leq f_{l-1} = b$. Solving Eq. (5) for $l \to (l - 1)$, we get allowed values of κ in an interval defined by b. Appending the above described procedure for the sequence of lower bounds of κ, we again find that for exactly one value of κ such that $a < b$, the vectors (a, b) and (b, a) belong to S_+. By the symmetry of the assumed initial configuration they also belong to S_-. Consequently, we proved rigorously the existence of a second type of NLE's, which are known as "odd-parity mode" [3]. Their characteristic feature is that the center of energy density of the solution is located on the lattice site $(l - 1)$ [10].

Due to the radius of interaction $r_0 = 1$, it follows that there are no other allowed stationary time-periodic NLE solutions with single-maximum amplitude distribution in lattices of type (3). In the limit $m \to \infty$ the two NLE solutions become compact and can be calulated analytically [8].

It would now be very interesting to analyze the map (5) in order to observe the previously discussed stable and unstable manifolds, and, consequently, the homoclinic points. However, this map (5) is not linearizable around the fixed point $f_l = 0$; some matrix elements of the Jacobian diverge. Consequently, it is impossible to determine the structure of the manifolds near the fixed point numerically. In order to proceed we add to the right hand side of (5) the terms,

$$C(f_l + f_{l-1}) + C(f_l + f_{l+1}) \ . \tag{6}$$

In this case, the modified map becomes linearizable around the fixed point $f_l = 0$. We can then visualize the manifolds, and hope that in the limit $C \to 0$ the structure of the manifolds does not change with respect to their intersections. In Fig. 2, we show the stable and unstable manifolds for $m = 2$, $C = 2$, and $\kappa = 10$, where we used the variables $g_l = f_l + f_{l-1}$ instead of the original ones. We computed the unstable manifold using the standard procedures [13] and indicated the position of the stable manifold as it can be evaluated out of the linearization around the fixed point. Clearly the horseshoe patterns are visible together with the homoclinic points. If one chooses one homoclinic point and iterates, then the image is the next-to-next homoclinic point. Consequently, if we would number all homoclinic points along the separatrix with integers in the order of their appearance (1,2,3,...), then a homoclinic point with an odd number will be mapped again into homoclinic points with odd numbers only (same for even numbers). Thus, we indeed observe the two possible even- and odd-parity solutions. The presence of additional NLE solutions would be indicated by a different mapping pattern of the homoclinic points. Moreover, from this result, it also follows that additional exact NLE solutions with a (presumably) irregular distribution of amplitude maxima do exist. The reason is that (5) is invertible—consequently the stable manifold in Fig. 2 will also show up with whiskers and horseshoe patterns (not shown in Fig. 2). The intersections of the whiskers of the stable and unstable manifolds are homoclinic points again and thus yield by definition

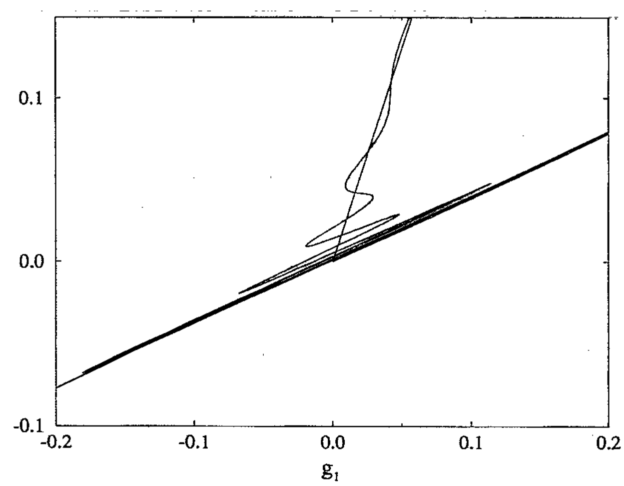

FIG. 2. Appearance of the homoclinic points and horseshoe structure for the perturbed map (5),(6) with variables as given in the text.

NLE solutions. In [9] analogous multisite NLE's were obtained as a consequence of the anti-integrability limit ideas of Aubry [16].

If we lower the value of C, then it becomes increasingly harder to find the unstable manifold. Still the structure of the unstable manifold can be seen partially, which indicates the persistence of the horseshoe patterns in phase space regions where the linear terms (6) are small perturbations. Then we can use the results of Sec. II and conclude that NLE solutions will survive under perturbations of the considered system. In particular, it follows that NLE's are exact solutions for Fermi-Pasta-Ulam chains with additional linear and cubic spring forces, as often studied in the literature [1, 4].

IV. CONCLUSION

In conclusion, we have shown that if a one-dimensional system is known, where NLE solutions exist and obey the nonresonance condition, then they are stable under perturbations of the Hamiltonian of the system or they can be perturbed in such a way that they become stable. Consequently, we can use exact proofs of the existence of NLE solutions, e.g., the one given in this work for (3) or the one in [9] and obtain NLE solutions for the corresponding perturbed system. Remarkably we are not restricted in the choice of the perturbation as long as the map for the perturbed system has the same phase space dimension.

Let us discuss the problems of the presented approach which appear when we try to consider lattices of dimensionality higher than $d = 1$. We can still make the ansatz of an existing time-periodic NLE solution and will yield again a coupled set of algebraic equations for the Fourier coefficients. However this set cannot be viewed as a discrete map of a certain phase space of the Fourier components, if $d > 1$. Consequently, we do not know how to formulate the conditions of the decay of the solution at infinity by imposing certain constraints on the set of equations. Still it is well known from numerical simulations that periodic NLE's exist [15].

Note added in proof. We have become aware recently of publications where the separation ansatz $X_l(t) = A_l G_l(t)$ for (3) was also proposed [17,18]. However, no proofs of the existence of NLE's were derived.

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