On the existence of localized excitations in nonlinear Hamiltonian lattices

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ABSTRACT

We consider time-periodic nonlinear localized excitations (NLEs) on one-dimensional translationally invariant Hamiltonian lattices with arbitrary finite interaction range and arbitrary finite number of degrees of freedom per unit cell. We analyse a mapping of the Fourier coefficients of the NLE solution. NLEs correspond to homoclinic points in the phase space of this map. Using dimensionality properties of separatrix manifolds of the mapping we show the persistence of NLE solutions under perturbations of the system, provided NLEs 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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1 Introduction

The existence, stability and properties of nonlinear localized excitations (NLEs) in Hamiltonian lattices with discrete translational symmetry have been subjects of growing research interest (see e.g. [1], [2], [3], [4] and references therein). NLEs can be viewed as generalized discrete analogs to the breather solution in a sine-Gordon equation [4]. 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 groundstate [5], [6].

There are a few known rigorous NLE existence proofs. First NLEs are exact solutions of the integrable Ablowitz-Ladik lattice [7]. In fact they form a three-parameter family of solutions. Secondly NLEs are exact solutions for the Fermi-Pasta-Ulam chain with box-like interaction potential [8]. In this case the NLEs are of compact support. Finally, and most importantly, MacKay and Aubry have derived an existence proof for NLEs 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 NLEs 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.

2 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 groundstate (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 groundstate (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.

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:

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

Then one can avoid resonance conditions of multiples of the fundamental frequency $\omega_1$ (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 NLEs requires the excitation of at least a second fundamental frequency in the ansatz (1), we can exclude them from the consideration and search for stationary time-periodic NLEs 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 NLEs 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

$$\vec{X}_l = \sum_{k=0, \pm 1, \pm 2, \ldots} \vec{A}_{(l,k)} e^{i\omega_1 kt}. \quad (2)$$

Now we can insert this ansatz (3) 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 (3) 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 (3) 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. Secondly 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 groundstate) 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 to an arbitrary phonon frequency of the linearized lattice equations, then it follows that the corresponding linear submap is characterized by a matrix $M_k$ of dimension $d_s \times d_s$ with $\det M_k = 1$ and $\lambda_i \lambda_{i+d_s} = 1$ where $\lambda_{i,i+d_s}$ are two of the $2d_s$ eigenvalues of $M_k$. Since these properties do not depend on the specific value of the considered phonon frequency, it follows that they are independent on $\tilde{\omega}$ and thus independent on $k$ and $\omega_1$. 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 of 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 $M_k$ are real and of 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 $d_{sm} = r_0 n_0$.

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 then a homoclinic point [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 cor-
responds to a set of homoclinic points of type i) then any small perturbation of the system will smoothly transform the NLE solution into a new 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 new 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 can not span the whole phase space of the map. Consequently there will be always 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 be never 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.

3 Proof of existence of NLE solutions for Fermi-Pasta-Ulam chains

In the last 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:

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

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 $A_l$:

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

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

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

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

First we note that for any value of $\kappa$ the map (5) has a fixed point $\vec{f}_{fp1} = (0, 0)$. Adding weak harmonic nearest neighbour 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 \((\mathbb{F})\). 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 $l \to \pm \infty$. Secondly 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 $\tilde{\kappa} = 2/(2m - 1)$.

Let us mention another useful property of the map \((\mathbb{F})\), which holds due to the discrete translational symmetry of the considered system \((\mathbb{F})\). If we generate a sequence of $f_2, f_3, \ldots$ starting with a vector $\vec{f}_1 = (a, b)$ and iterating \((\mathbb{F})\) towards growing integers $l$, then we can generate the same sequence of numbers by iterating \((\mathbb{F})\) 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 $\kappa$ is confined to $\kappa^- \leq \kappa \leq \kappa^+$ with $\kappa^- = (\kappa f_{l+1} + f_l^{2m-1})/f_l$ and $\kappa^+ = \kappa^- + (2^{2m-1} - 1)f_l^{2m-2}$. 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 $\kappa$ 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 $\kappa^+_{l+1} \leq \kappa^+$. Because $c$ is a monotonic function of $\kappa$ we can satisfy $a \geq f_{l+1} \geq f_{l+2} \geq 0$ only if $\kappa^- \leq \kappa \leq \kappa^+$ for $a = b$ and $\kappa^- < \kappa < \kappa^+$ for $a < b$. Repeating this procedure for every following lattice site we get a sequence of monotonically increasing lower bounds on $\kappa$ defined by the vanishing of $f_{l+m} = 0$ in the $m$-th step. In the limit $m \to \infty$ we thus obtain exactly one value of $\kappa$, which is the limit of the mentioned sequence of lower bounds. This limiting value is finite, because it is always smaller than $\kappa^+$. It can not be equal to $\kappa^+$ 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 $\kappa$ 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 $\kappa$ 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 NLEs, 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 the equation (5) for \(l \to (l - 1)\) we get allowed values of \(\kappa\) in an interval defined by \(b\). Appending the above described procedure for the sequence of lower bounds of \(\kappa\) we again find that for exactly one value of \(\kappa\) 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 NLEs, 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 in lattices of type (3). In the limit \(m \to \infty\) the two NLE solutions become compact and can be calculated analytically [8]. It would be now very interesting to analyse 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

\[ C(f_l + f_{l-1}) + C(f_l + f_{l+1}) \]  

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 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. Thus we indeed observe the two possible even and odd parity solutions. 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 are small perturbations. Then we can use the results of Section II and conclude that NLE solutions will survive under perturbations of the considered system. In particular it follows that NLEs are exact solutions for Fermi-Pasta-Ulam chains with additional linear and cubic spring forces, as often studied in the literature [1], [4].

4 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 [3] and obtain new 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 can not 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 NLEs exist [5].

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References

[1] A. J. Sievers and S. Takeno. Phys. Rev. Lett. 61, 970 (1988).

[2] D. K. Campbell and M. Peyrard. in: CHAOS - Soviet American Perspectives on Nonlinear Science, ed. by D. K. Campbell. American Institute of Physics New York, 1990.

[3] J. B. Page. Phys. Rev. B41, 7835 (1990).

[4] S. Takeno. J. Phys. Soc. Japan 61, 2821 (1992).

[5] S. Flach, C. R. Willis, and E. Olbrich. Phys. Rev. E 49, 836 (1994).

[6] S. Flach. Phys. Rev. E, in press (October 1994).

[7] M. J. Ablowitz and J. F. Ladik. J. Math. Phys. 17, 1011 (1976).

[8] K. W. Sandusky, J. B. Page, and K. E. Schmidt. Phys. Rev. B46, 6161 (1992).

[9] R. S. MacKay and S. Aubry. Warwick Report No. 20/1994, unpublished (1994).

[10] S. Flach and C. R. Willis. Phys. Rev. Lett. 72, 1777 (1994).

[11] J. Denzler. Commun. Math. Phys. 158, 397 (1993).

[12] V. M. Eleonskii, N. E. Kulagin, N. S. Novozhilova, and V. P. Shilin. Teor. Mat. Fiz. 60, 395 (1984).

[13] A. J. Lichtenberg and M. A. Lieberman. Regular and Stochastic Motion. Springer, New York, 1992.

[14] Yu. S. Kivshar. Phys. Rev. E 48, R43 (1993).

[15] S. Flach, K. Kladko, and C. R. Willis. Phys. Rev. E , in press (September 1994).
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).

Fig. 2

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