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# LOCALIZED OSCILLATIONS IN NONLINEAR LATTICES : EXISTENCE AND STABILITY

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**Abstract.** *Numerical methods using homoclinic orbits are applied to study the existence and stability of spatially localized and time-periodic oscillations of 1-dimensional (1D) nonlinear lattices, with linear interaction between nearest neighbors and a quartic on – site potential*

$$V(u) = \frac{1}{2}Ku^2 \pm \frac{1}{4}u^4$$

*where the ( + ) sign corresponds to "hard spring" and ( - ) to "soft spring" models. These localized oscillations - when they are stable under small perturbations - are very important for physical systems, since they seriously affect the energy transport properties of the lattice. We use Floquet theory to analyze their linear (local) stability, along certain curves in parameter space (α, ω), where α is the coupling constant and ω the frequency of the breather. We then apply the Smaller Alignment Index method (SALI) to investigate more globally their stability properties in phase space. Comparing our results for the ± cases of V(u), we find that the regions of existence and stability for simple breathers of the "hard spring" lattice are considerably larger than those of the "soft spring" system. The variation of the size of the regular region around a stable breather is investigated as the number of particles is increased.*

## 1 INTRODUCTION

We consider a one – dimensional (1D) lattice described by the equations of motion:

$$\ddot{u}_n + V'(u_n) = a(u_{n+1} + u_{n-1} - 2u_n) \quad , \quad -\infty < n < +\infty \ , \tag{1}$$

where $u_n(t)$ is the displacement of the particle at nth lattice site, $a$ the coupling parameter and $V(u)$ and on - site potential given by the form:

$$V(u) = \frac{1}{2}Ku^2 \pm \frac{1}{2}u^4 \quad , \tag{2}$$

where K > 0 is a fixed parameter. Dots indicate time derivatives, and primes differentiation with respect to the argument. These equations describe the dynamics of an infinitely long chain of oscillators, each linearly coupled to its nearest neighbors and experiencing a “substrate” potential *V.* The (+) sign in Eq. (2) implies that the particles are tied to the substrate by “hard spring” forces, while the (–) sign refers to the “soft spring” case. Since the seminal paper of MacKay and Aubry in 1994 [1], in which the existence of localized, time periodic solutions (the so – called **discrete breathers**) of systems like (1) was rigorously established, there has been a wealth of results in the physics and mathematics literature, concerning the properties of these solutions (see e.g. [2-5]). There exist several methods to compute **numerically exact** breather solutions for system (1) with on site potential (2). With the term “numerically exact” breather, we mean a solution, which is time-periodic and spatially localized for a lattice of N particles and retains its shape as N is arbitrarily increased. For example, one can use the method of continuation starting from the limit $\alpha = 0$ , as explained e.g. in [1] and [4].

On the other hand, it is also possible to apply relaxation methods based on the fact that, if a breather solution exists and is stable, it should attract a region of phase space around it, assuming that some dissipative process is present to eliminate any excess energy [6-8]. In the present paper, we prefer to use the more recently developed method of **homoclinic orbits of invertible maps**, as described in [9] and implemented in [10-11], which turns out to be very convenient, as it can be applied independently of the value of the coupling parameter $a$ . This method operates in Fourier space and offers excellent approximations for breathers, which can be made “numerically exact” by using the convergence of Newton schemes to construct them to arbitrary accuracy. Furthermore, it provides a systematic way by which all types of breathers possessing an arbitrary number of “local extrema” (the so-called multibreathers) can be constructed. Finally our analytical predictions are fully confirmed by numerical simulations, which are presented in this paper and in detail in [12].

## 2 THE METHOD OF HOMOCLINIC ORBITS

Since a discrete breather solution of Eq.(1) is time-periodic with, say, period $T$ and frequency $\omega = 2\pi / T$ , it can be expanded in Fourier series

$$u_n(t) = \sum_{k=-\infty}^{\infty} A_n(k) \exp(ik\omega t) \quad , \tag{3}$$

with coefficients

$$A_n(k) = A_n^*(-k). \tag{4}$$

Since the oscillations are expected to have zero mean, by virtue of the form of the potential (2), we set $A_n(0)=0$. Furthermore, all particles oscillate in phase, hence we may search for solutions with initial velocities zero, thus taking all the $A_n(k)$ to be real numbers. Finally, due to the symmetry of the on site potential (2), only the modes with odd index $k$ , i.e. $k = 1,\ 3,\ 5...$, are non-zero. The existence of such periodic solutions for “hard spring” systems (with + in (2)) has already been extensively demonstrated in the recent literature [9-11]. In this paper, we shall concentrate on the **“soft spring”** potential

$$V(u) = \frac{1}{2} K u^2 - \frac{1}{2} u^4 \ . \tag{5}$$

Inserting Eq. (3) in the equations of motion (1) and equating coefficients of $\exp(ik\omega t)$ for every $k$ , we obtain the following algebraic system for the $A_n(k)$ :

$$A_{n+1}(k) + A_{n-1}(k) = C(k) A_n(k) - \frac{1}{\alpha} \sum_{k_1} \sum_{k_2} \sum_{k_3} A_n(k_1) A_n(k_2) A_n(k_3) \quad , \tag{6}$$

where $k_1 + k_2 + k_3 = k$ and

$$C(k) = \left( 2 + \frac{K - k^2 \omega^2}{\alpha} \right). \tag{7}$$

The recurrence relation (6) is an infinite-dimensional mapping of the Fourier coefficients $A_n(k)$ with lattice site index n as iteration parameter. Spatial localization requires that the Fourier amplitudes in the recurrence relation (6) satisfy $A_n(k) \to 0$ as $\|n\| \to \infty$. Hence a discrete (multi-) breather is a **homoclinic orbit** in the space of Fourier coefficients, i.e. a doubly infinite sequence of points beginning at 0 for $n \to -\infty$ and ending at 0 for $n \to \infty$. Of course, in any numerical method the index space $(n,k)$ has to be restricted to a finite subspace. Following the above arguments, if the Fourier series of Eq.(4) converges, the $|A_n(k)|$ diminish rapidly with increasing $|k|$, hence it is sufficient to consider only a small number of harmonics of Fourier series in Eq.(4), say M, for all n lattice sites ($-\infty < n < +\infty$), i.e. $k = 1, 2, ..., M$. Under these conditions, Eq.(6) represents a 2M-dimensional map and spatially localized time-periodic solutions may be expected to exist in the neighborhood of the trivial solution ($A_n(k) = 0$, for all n, k), provided this solution is hyperbolic, i.e. represents a **saddle point** of the map. The requirement that the fixed point of the 2M-dimensional map is hyperbolic (saddle point), with an M-dimensional stable and an M-dimensional unstable manifold, is filled if we require:

$$\omega^2 k^2 < K \text{ or } \omega^2 k^2 > K + 4\alpha \tag{8}$$

where $\omega$ is the if the fundamental frequency $\omega$, obtained from Eq.(7), with k=1:

$$\omega = \sqrt{K - \alpha(C(1) - 2)} \tag{9}$$

Thus, breathers exist if the fundamental frequency $\omega$ and all its harmonics have values outside the range (K, K+4α) specified by (8). This range, in fact, represents the spectrum of **linear modes** of the particles (the so – called **"phonons"**) and is often called the **propagation zone**, since it is within this range of frequencies that small disturbances can propagate along the lattice. If $\omega k$ were to lie in this range for some k, this would imply **the reduction of dimensions** of the unstable manifold. Thus, the origin could not be a saddle fixed point of map (6) and homoclinic points (and breather solutions) would not exist with equivalent properties as $n \to \pm\infty$.

Let us consider now the simplest possible approximation, for which the Fourier series (3) is represented by a single mode only, i.e.

$$u_n^{(0)}(t) = 2A_n(1)\cos\omega t\ ,\ -\infty < n < +\infty. \tag{10}$$

Substituting Eq. (10) into Eq. (1), using Eq. (2), and scaling also the Fourier coefficients by

$$A_n(1) = \sqrt{\alpha}\ \ A_n\ , \tag{11}$$

we obtain finally

$$A_{n+1} + A_{n-1} + C(1)A_n = -3A_n^3\ , \tag{12}$$

where

$$C(1) = \left(2 + \frac{K - \omega^2}{\alpha}\right). \tag{13}$$

Thus, instead of studying the 2M-D map (6), we solve the 2-D map (12) to obtain "zeroth" order approximations (10) of the breather solutions of the 1-D lattice (1) with the quartic on site potential (2). Clearly, the fixed point (0,0) of the 2-D map (12) will be hyperbolic, with a 1-D stable and a 1-D unstable manifold, if C(1) > 2 or C(1) < -2. For the case of "soft spring" we only treat here the case C(1)> 2, because for C(1)< - 2 the invariant manifolds of the saddle point at (0,0) do not intersect and breathers are not expected to exist. Using (15), the inequality C(1) > 2 means that the value of the frequency $\omega$ is below the phonon band (propagation zone), i.e $\omega^2 < K$.

Thus, to have breather solutions, one must appropriately restrict the system's parameters so that the frequencies of all harmonics, $k\omega$, lie **outside** the phonon band (K, K+4α). By comparison, the values of the frequencies (fundamental and harmonics) of the "hard spring" system are **all above** the phonon band, once $\omega^2 > K + 4\alpha$ is satisfied. Consequently, the parameter range for the existence of breathers of the "hard spring" lattice is **much larger** than the corresponding one for the "soft spring" potential (5).

An orbit is also referred to as a solution of the map, since it solves the system of equations (12). Orbits considered in this paper are orbits connecting the saddle point (0,0) of our map to itself and are called **homoclinic orbits**. A homoclinic orbit consists by definition of states $\mathbf{x}_n$, which lie at the intersection of unstable manifold and stable manifold of the saddle fixed point. If there is one state for which this holds, there exist infinitely many of them, thus giving rise to an infinity of homoclinic orbits. The emerging picture is that of *a* **homoclinic tangle**. An example of such a structure is shown in Fig.1, where we plot in the $A_{n+1}, A_n$ plane the stable and unstable manifolds of the saddle point at (0,0) of two-dimensional map Eq.(12) with C(1)=3.

## 2 LOCAL AND GLOBAL STABILITY OF DISCRETE BREATHERS

The time-periodic solution $\{u_n(t)\}$ of eq.(1) with per site potential Eq.(2) is called **linearly stable** when all the eigenvalues of Floquet matrix lie on the unit circle. When some eigenvalue pairs "split off" the unit circle then the corresponding perturbations grow exponentially in time and the breather is called **linearly unstable**. (For a discussion of all these concepts concerning the linear stability of discrete breathers see [5].

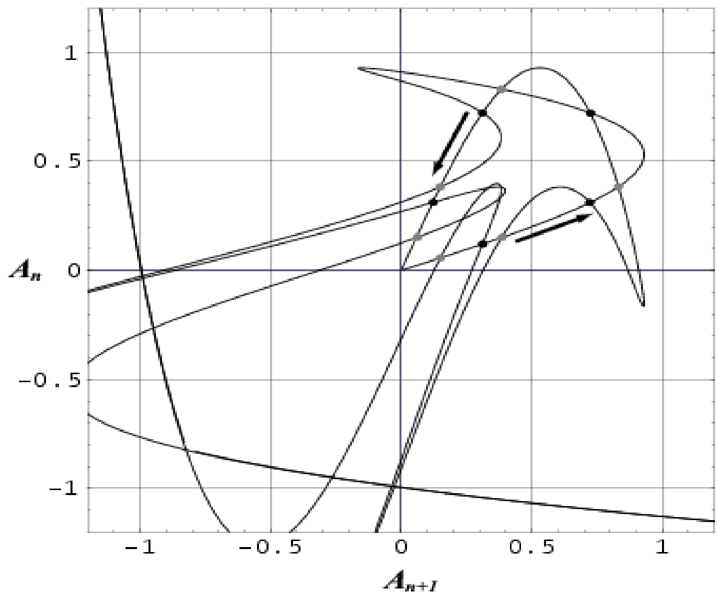


Figure 1. Part of the homoclinic tangle around the origin of the map of Eq. (12) at C(1) = 3. The stable and manifolds are the curves emerging out of the (0,0) saddle point. Some points of two homoclinic orbits at their intersections (corresponding to two different breather solutions), are shown by dark and gray dots respectively. They provide very accurate estimates for the oscillation amplitudes An of the particles of the lattice, $n \in \mathbb{Z}$.

Using the method of homoclinic orbits described above, we have constructed a large number of breather solutions of Eq.(1) with the potential (5) and studied their linear stability characteristics. We thus obtained the following results:

- In most cases, as the coupling parameter α increases, breather solutions for 'soft spring' systems undergo a **complex instability** transition, i.e. a complex conjugate pair of their eigenvalues achieves magnitudes larger than one by splitting off the unit circle in two complex conjugate pairs (see Fig.3(c)). It is important to note that **unlike other bifurcation types** (like pitchfork, period – doubling etc.), this instability transition represents the termination of a family of periodic solutions, as it is not associated with the simultaneous appearance of other (stable) periodic solutions [19, 20].
- Unlike the hard spring case, when we follow curves in the parametric space (α,K,ω), described by the function:

$$G(a,K,\omega) = -\left(2 + \frac{K-\omega^2}{a}\right) = \text{const.} \quad , \tag{14}$$

breather solutions for “soft spring” systems **do not preserve** the number of eigenvalues of the Floquet matrix with absolute values different from one. In Fig.2 we depict the distribution of eigenvalues of the monodromy matrix for a “soft spring” breather solution for various values of coupling parameter $a$, keeping constant the values for $C(1)$ for $K$ (see Eq. (13)).

By comparison, the breather solutions of systems (1) with quartic “hard spring” potential do not appear to exhibit complex instability transitions, as they are always found to become unstable by pairs of eigenvalues splitting off the unit circle at +1 on the real axis. Furthermore, they do possess curves in parameter space (α, K, ω), described approximately by Eq.(14), along which breather solutions do not change their stability preserving the number of eigenvalues of monodromy matrix with absolute values different from one .

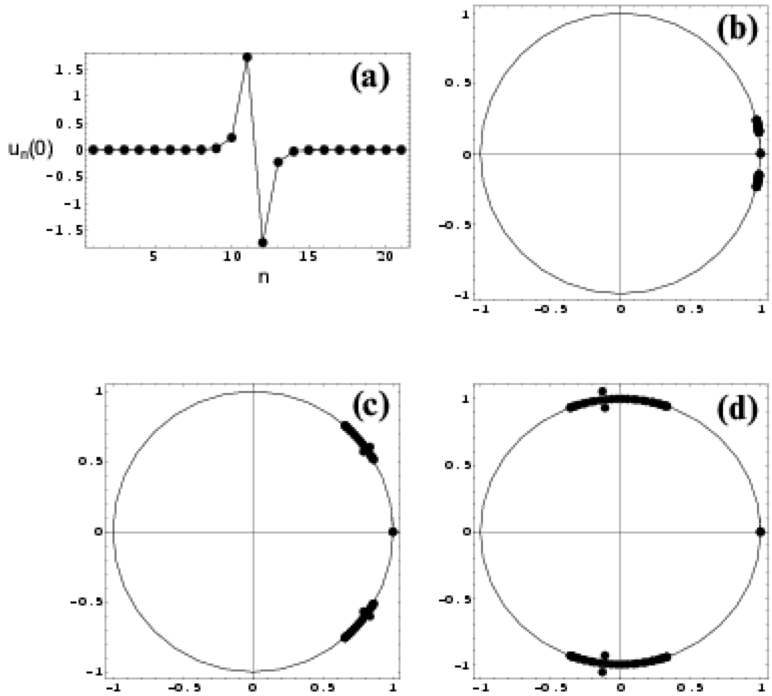


Figure 2. For the “soft spring” breather shown in (a), with 21 particles and C(1)=8, K=2, we display in the complex plane how the distribution of the eigenvalues of the monodromy matrix changes as the coupling parameter α is increased: (b) α=0.015, (c) α=0.05 and (d) α=0.1. Note the occurrence of complex instability at $\alpha \geq 0.05$.

A more “global” investigation of the stability of discrete breathers can be performed using the method of the Smaller Alignment Index (SALI) to discriminate between ordered and chaotic motion in a very efficient way. This method was introduced in [13], where it was applied successfully in 2D, 4D and 6D symplectic maps. More importantly, however, it distinguishes order from chaos also in Hamiltonian systems, as shown in [14-17], where it was applied to systems with 2 and 3 degrees of freedom. The main advantage of the SALI is that it has completely different behavior for ordered and chaotic orbits, which allow us to decide the nature of the orbit faster than other traditional methods, like e.g. the computation of Lyapunov characteristic exponents. In particular the SALI fluctuates around non-zero values for ordered motion, while it goes abruptly to zero for chaotic orbits. In the latter case, the SALI can also reach the limit of the accuracy of the computer ($10^{-16}$), which means that the chaotic nature of the orbit is established beyond any doubt and no further computations are needed. In order to compute the SALI we follow simultaneously the evolution of orbit and **two initially different deviation vectors** $v_1(0)$, $v_2(0)$. In every iteration $N^*$ the deviation vectors are normalized keeping their norm equal to 1, while the norm of their sum (antiparallel alignment index, $ALI_+$) and their difference (parallel alignment index, $ALI_-$) are also computed. Then the SALI is defined as the minimum of these two quantities:

$$\mathrm{SALI}(N^*) = \min\left\{ \left\| \frac{v_1(N^*)}{\|v_1(N^*)\|} + \frac{v_2(N^*)}{\|v_2(N^*)\|} \right\|, \left\| \frac{v_1(N^*)}{\|v_1(N^*)\|} - \frac{v_2(N^*)}{\|v_2(N^*)\|} \right\| \right\}, \qquad (15)$$

with || . || denoting the euclidean norm.

In the case of chaotic orbits the two deviation vectors will eventually be aligned with the most unstable direction [13], becoming equal ($ALI_-$=0) or opposite ($ALI_+$=0), which means that the SALI becomes zero. In the case of ordered orbits on the other hand, the motion is **quasiperiodic** and takes place on a torus, as if the system were integrable. Thus, any pair of arbitrary deviation vectors tend to the tangent space of the torus and since there is no reason why they should become aligned, in general, they oscillate about two different directions and **the SALI fluctuates around some non-zero value**. In [17] the behavior of the SALI for ordered orbits was studied and explained in detail in the case of a completely integrable 2D Hamiltonian system. In the present paper we have applied the SALI method to find out how **persistent** is the ordered behavior around stable breathers in the hard and soft spring potentials.

Of course, since the numerically exact breathers correspond to periodic orbits in a multidimensional phase space, they can be perturbed by changing a number of different variables. In order to get a rough idea of the 'size' of the phase space region of ordered behavior around the stable breather we have chosen to perturb only the initial position of the central particle $u_0$.

So, starting from the stable periodic orbit and changing $u_0$ we compute for a sample of orbits the SALI using as initial deviation vectors $v_1(0)$ = (1,0,…..0), $v_2(0)$= (0,1,0,…,0). The SALI of ordered orbits remains always different from zero exhibiting some small fluctuations. This behavior is shown in the log-log plots of Fig. 3 for the soft spring potential and Fig. 4 for the hard spring case, where the SALI of a stable periodic orbit is plotted as function of the number of iterations $N^*$ (curves (a) in both figures).

In the soft spring case, the first chaotic orbit was found for a perturbation $\Delta u_0$=0.2207 and the evolution of the corresponding SALI is plotted in Fig. 3 as curve (b). We see that after an initial transient time interval the SALI decreases abruptly reaching very small values, $10^{-10}$ after $N^* \approx 1500$ iterations, which is the typical behavior of the SALI for chaotic motion. On the other hand, in the hard spring case it is much **harder to destabilize** the stable periodic orbit as we need a considerably higher perturbation $\Delta u_0$ to have chaotic motion. In particular we have to perturb the position of the central particle by $\Delta u_0$=1.3 to get a chaotic orbit, the SALI of which is plotted in Fig 4 as curve (b). Again we have an abrupt fall of the SALI to very small values reaching $10^{-10}$ after $N^*$ = 9500 iterations.

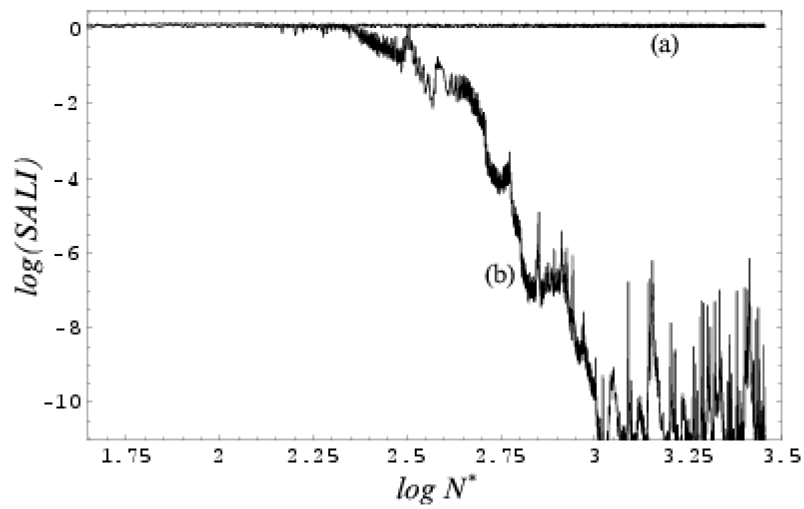


Figure 3. The log-log evolution of SALI with respect to the number $N^*$ of iterations for the stable breather solution with soft spring potential containing 21 particles at C(1)=8, α=0.15275, K=2 (curve (a)) and for the same orbit with a perturbation $\Delta_{u0}$=0.2207 in the initial position of the central particle (curve (b)).

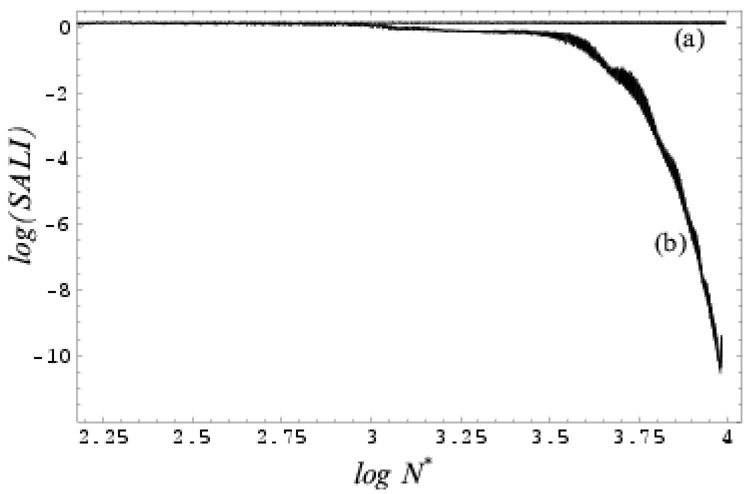


Figure 4. The log-log evolution of the SALI with respect to the number $N^*$ of iterations for a stable breather with hard spring potential containing 21 particles at C(1)=8, α=0.15275, K=2 (curve (a)) and for the orbit with a perturbation $\Delta_{u0}$=1.3 in the initial position of the central particle (curve (b)).

## 6 CONCLUSIONS

Our main results can thus be summarized as follows: In a one dimensional lattice with on site potential describing a "hard spring" and a "soft spring system", varying the lattice coupling parameter α > 0, we have studied bifurcations of **localized periodic solutions** (called "breathers") and have found that the "hard spring" breathers preserve their stability over much longer parameter intervals and upon bifurcations inherit their stability to new breathers. The "soft spring" breathers on the other hand, very often undergo **complex instability** transitions, at which no new periodic solutions arise. We have also used the SALI method to examine the presence of ordered or chaotic motion **more "globally"** in the vicinity of a breather in its multidimensional phase space. Thus, we have observed that regions of **regular motion** around stable breathers **are considerably larger** and evidence of **chaotic behavior** is observed **significantly further** from them in the **"hard spring" lattice**, in comparison with similar results for the **"soft spring" system**.

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