EXISTENCE AND PROPERTIES OF DISCRETE BREATHERS

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Nonlinear classical Hamiltonian lattices exhibit generic solutions in the form of discrete breathers. These solutions are time-periodic and (at least) exponentially localized in space. The lattices exhibit discrete translational symmetry. Discrete breathers are not confined to certain lattice dimensions. Necessary ingridients for their occurence are the existence of upper bounds on the linear spectrum (of small fluctuations around the groundstate) of the system as well as the nonlinearity. I will present existence proofs, formulate necessary existence conditions, and discuss structural stability of discrete breathers. The following results will be also discussed: the birth of breathers through tangential bifurcation of band edge plane waves; dynamical stability; details of the spatial decay; numerical methods of obtaining breathers; interaction of breathers with phonons and electrons; movability.

1 Introduction

It is well-known that nonlinear media support localized energetical excitations. For integrable nonlinear systems these solutions are the conventional solitons.[a] These solutions have energies larger than the state of lowest energy of the system (thus we coin them excitations). Most of the studies are usually done for systems with a continuous translational symmetry (field equations). If the considered system is allowed to evolve in time according to some dynamical equations of motion, then besides stationary static localized solutions (and the family of related solutions which are generated by the corresponding symmetry of the system) also time-dependent stationary localized solutions may exist. A well-known member of the latter group is the breather solution of the sine-Gordon (sG) equation in 1+1 dimensions. It is this type of solutions we will deal with in the following, although the final results might be well applicable to other (but similar) types of solutions too.

1.1 Some Properties of Breathers in Hamiltonian Field Equations

Let us characterize sG breather solutions with respect to the considerations to follow. The sG equation for a field $\Psi(x,t)$ is a particular example out of the

[a] For nonintegrable systems there seems to be no unique definition of those solutions.

class of nonlinear Klein-Gordon (KG) equations

$$\Psi_{,tt} = C\Psi_{,xx} - F(\Psi) \tag{1}$$

with the choice $F_{sG}(z) = \sin z$. The breather solution is given by

$$\Psi_b(x,t) = 4\tan^{-1}\left[\frac{m}{\omega}\frac{\sin(\omega t)}{\mathrm{ch}(mx)}\right] \ , \ \omega = \sqrt{1-m^2}. \tag{2}$$

It represents a field which is periodically oscillating in time and decays exponentially in space as the distance from the center $x = 0$ is increased.

Most probably these breather solutions are *nongeneric*. This statement is due to the following facts. Birnir showed [1] that sG breathers are *isolated*, i.e. the solutions survive only under a finite number of perturbations $\delta(z)$ of $F_{sG}(z) \to F_{sG}(z) + \delta(z)$. Years of searching for breathers in ϕ^4 systems ($F(z) = -z + z^3$) were terminated by the nonexistence proof of breathers by Segur and Kruskal [2]. Finally we are not aware of existence proofs of similar solutions in 1+2 dimensions. So we deal up to now with structurally unstable solutions, which are not interesting for most of the possible applications. The reason for that lies in the fact that a decomposition of (2) into a Fourier series with respect to time yields higher harmonics with frequencies $k\omega$ (k is the Fourier number). These frequencies resonate with the linear spectrum of (1) $\omega_q = \sqrt{Cq^2 + F'(z=0)}$ (q - wave number), if k is larger than a given number which depends on the choice of ω. Consequently the corresponding separatrix manifolds associated with (1) are of finite dimension. Together with the infinity of the dimension of the corresponding phase space the structural instability follows immediately [3].

1.2 The Lattice Case

Now let us consider a lattice, which is obtained from say (1) by replacing the continuous x-axis with an equidistant set of points labeled with l, and by replacing the second derivative with respect to x in (1) with a second difference. In a more general fashion the system can be described by the following Hamilton function:

$$H = \sum_l \left[\frac{1}{2}\dot{X}_l^2 + \Phi(X_l - X_{l-1}) + V(X_l)\right]. \tag{3}$$

Here $\dot{A}$ denotes a time derivative, and the equations of motion are given by $\ddot{X}_l = -\partial H/\partial X_l$. The main change by going over from (1) to (3) is the change of continuous translational symmetry to discrete translational symmetry. This reduction of symmetry has several consequencies for the dynamics of the system. The potential functions $V(z)$ and $\Phi(z)$ can be expanded around the energy minimum:

$$V(z) = \sum_{\mu=2,3,..} \frac{v_\mu}{\mu} z^\mu \ , \ \Phi(z) = \sum_{\mu=2,3,..} \frac{\phi_\mu}{\mu} z^\mu . \tag{4}$$

The linear spectrum is now given by $\omega_q^2 = v_2 + 4\phi_2 \sin^2(\pi q/2)$. As opposed to (1) the linear spectrum of (4) is *bounded* from above : $v_2 \leq \omega_q^2 \leq (v_2 + 4\phi_2)$. Clearly this can change the properties of the mentioned separatrix manifolds drastically. Systems of the type (3) are the simplest realizations of models widely used in many areas of physics, as e.g. solid state physics, arrays of Josephson junctions etc, where the discreteness of the system plays an important role.

2 Discrete Breathers

Let us search for spatially localized and time-periodic solutions of (3) which can be coined discrete breathers due to the similarity to the sG breather solutions. The required periodicity in time allows to expand the ansatz in a Fourier series:

$$X_l(t) = \sum_{k=-\infty}^{+\infty} A_{kl} \mathrm{e}^{\mathrm{i}k\omega t} \ , \ A_{k,l\to\pm\infty} \to 0. \tag{5}$$

2.1 Necessary Existence Condition

Inserting this ansatz into the equations of motion and eliminating time we arrive at a nonlinear coupled set of algebraic equations for the coefficients A_{kl} [4]. This set can be rewritten as a map

$$A_{k,(l+1)} = M(\{A_{k'l}\}, \{A_{k',(l-1)}\}). \tag{6}$$

M has a fixed point $A_{kl} = 0$. Linearizing M around this fixed point we obtain[b]

$$A_{k,(l+1)} = [2\kappa_k + 2]\, A_{kl} - A_{k,(l-1)} \ , \ \kappa_k = \frac{v_2 - k^2\omega^2}{2\phi_2} . \tag{7}$$

The fixed point $A_{kl} = 0$ of (7) is an elliptic one if $k\omega = \omega_q$ and a hyperbolic one if $k\omega \neq \omega_q$. Since only the hyperbolicity of the fixed point suites the required

[b]There are limitations on the linearization procedure which apply when some multiple $k\omega$ comes too close to the linear spectrum [5].

spatial localization property of the ansatz (5) the necessary condition for the existence of a generic discrete breather is

$$k\omega \neq \omega_q. \tag{8}$$

Clearly we can satisfy this condition for a lattice[c] because the linear spectrum is bounded from above - in contrast to the continuous case, where condition (8) can be never fulfilled. The algebraic equations (6) can be solved numerically [5]. From (7) it follows that a discrete breather is characterized by an exponential decay in space with k-dependent exponents [4,5]:

$$A_{kl} \sim [\mathrm{sgn}(\lambda_k)]^l \, \mathrm{e}^{\ln|\lambda_k|l} \ , \ \lambda_k = 1 + \kappa_k \pm \sqrt{(1+\kappa_k)^2 - 1}, \tag{9}$$

where the sign has to be chosen such that $|\lambda_k| < 1$. Numerical solutions nicely reproduce those features [5].

In the limit of large values of k it follows $|\lambda_k| \approx \omega^2 k^2/\phi_2$ and consequently the k-dependence of A_{kl} is given by [5] $A_{kl} \sim k^{-2|l|}s(k)$, where $s(k)$ is a monotonous decreasing function with increasing k. Thus the decay of A_{kl} in the k-space is stronger than $k^{-2|l|}$ (here $|l|$ measures the distance from the center of the solution). This is one of the reasons why the Rotating Wave Approximation used by Takeno [6] and others (it amounts to neglecting all but the first Fourier component) often produces approximate solutions quite close to the exact ones.

2.2 Structural Stability

For the 1d lattice (where (6) applies) it is straightforward to conclude, that in the case of (8) a discrete breather is *structurally stable* [7]. This follows from the circumstance that if (8) applies for an existing discrete breather solution, the stable and unstable invariant manifolds of the fixed point $A_{kl} = 0$ of (6) have common homoclinic points and dimension half of the phase space dimension of map (6) [7]. Then either i) small perturbations of the Hamiltonian (3) preserve the existence of those homoclinic points (and thus the existence of a discrete breather) or ii) there exist 'right' perturbations such that the discrete breather becomes structurally stable in the vicinity of the new perturbed Hamiltonian.[d]

If the condition (8) is violated for a given number n of k-values, then the separatrix manifold dimensions are reduced by that number [7]. Consequently

[c] Note that for higher dimensional lattices one can find the same condition through an analysis of the corresponding linearized equations with the only difference that these equations do not constitute a map as in the 1d case.

[d] No analogous result is known for higher dimensions, because the problem can not be reduced to a map; still there is evidence that discrete breathers are structurally stable in higher dimensions too [8].

even if a discrete breather exists, it would be structurally unstable, since always $2n$ perturbations of (3) exist which destroy the solution. In the continuum limit $(C \rightarrow \infty)$ $n \rightarrow \infty$ for any finite ω, and thus no structurally stable breathers remain in the continuous case - in agreement with the results quoted in the introduction.

Further it follows [4], that no structurally stable localized solutions exist, with quasiperiodic time dependence. This steams from the fact that the condition (8) has then to be replaced by $k_1\omega_1 + k_2\omega_2 + ... + k_m\omega_m \neq \omega_q$, where the ratios of the frequencies ω_i are irrational. It is straightforward to show that there exists an infinite number of combinations $(k_1, k_2, .., k_m)$ such that the new condition is violated for any choice of the frequencies ω_i [4].

2.3 Existence Proofs

Up to now we know about two rigorous existence proofs for discrete breathers. MacKay and Aubry considered weakly coupled anharmonic oscillators, i.e. $V(z)$ anharmonic, $\Phi(z)$ small [9]. Then it is possible to show that time-periodic localized solutions of the trivial case $\Phi(z) = 0$ can be analytically continued into the weakly coupled regime if the condition $\omega/\sqrt{v_2}$ irrational is met. Remarkably this proof goes equally well for any lattice dimension, and is quite robust to variations in the interaction range.

The second proof is due to Flach and it considers a 1d system with homogeneous potentials [7]: $(V(\lambda z) + \Phi(\lambda z)) = \lambda^{2m}(V(z) + \Phi(z))$. Due to this additional symmetry discrete breather solutions have the form $X_l(t) = A_l G(t)$, i.e. space-time separability applies. The resulting two-dimensional map for A_l is analyzed and the existence of homoclinic points is shown to be true [7]. Note that this proof also incorporates the special case $V(z) = 0$, where only the interaction potential remains - in contrast to the weak coupling limit of the existence proof by MacKay and Aubry [9].

2.4 Dynamical Stability

If we perturb the trajectory of an exact discrete breather solution then it is important (with respect to applications) to know how long the new trajectory evolves closely enough to the old localized solution. In the previous chapter we have already shown that quasiperiodic breathers do not exist in general. Consequently a perturbed breather will be an object which radiates energy out of its center (because otherwise it would be a new non-periodic breather solution!). There exists no general approach to the problem of stability - actually in most of the nonintegrable systems we will run into the problem of small denominators and ultimate chaos. In a numerical investigation [10] perturbed breathers could either radiate a bit of energy and become essentially time-periodic again (and thus exact) or internal resonances could evolve, which eventually lead to chaotic motion *confined* to the breather volume. That chaotic motion leads to an increase in the radiation power of several orders of magnitude. Alltogether a rather complex scenario seems to evolve.

It is useful to linearize the equations of motion for the perturbation $\delta_l = X_l - X_l(t)$ (here $X_l(t)$ denotes the time-periodic breather solution):

$$\ddot{\delta}_l = - \left. \frac{\partial^2 H}{\partial X_l \partial X_{l'}} \right|_{X_l = X_l(t)} \delta_{l'} . \tag{10}$$

These equations are a generalization of Hill's equation [11]. The problem amounts to diagonalizing a matrix. Since the breather is a localized solution, one can immediately state that all extended eigenvectors have frequencies of the linear spectrum. Consequently time-periodic breathers are stable with respect to small amplitude phonon perturbations if the condition $k\omega \neq 2\omega_q$ is fulfilled [10]. Note that this stability condition includes the already obtained existence condition (8). The localized eigenvectors (and their corresponding eigenvalues) have to be found through numerical diagonalizations.

2.5 Breather Birth due to Band Edge Phonon Bifurcations

For small systems (few degrees of freedom) and small amplitudes/energies the phonon orbits are surely stable. So breathers have to occur through certain bifurcations of the linear orbits. The analysis of stability of band edge phonons has been done in a recent work [12]. The result is that for large systems only the first six expansion coeffiecients of the potentials have to be known: $v_2, v_3, v_4, \phi_2, \phi_3, \phi_4$. Then the phonon orbit is characterized by a nonnegative energy. The phonon orbit becomes unstable at a bifurcation energy $E_c \sim N^{-2/d}$ where N is the size of the system and d the dimensionality. The proportionality factor is required to be positive. This condition is in most of the cases equivalent to the condition that *the frequency of the band edge phonon orbit is repelled from the linear spectrum with increase in energy*. The new bifurcating periodic orbits are shown to be *not* invariant under the discrete translational symmetry of the system. These new orbits eventually become discrete breathers [12].

2.6 Movability

It is possible to create moving discrete breathers [13]. We remind the reader that this is nontrivial due to the low symmetry of the lattice as compared to a field equation. Up to now there exist no proofs of existence of moving breathers. All reports refer to numerical simulations with finite simulation time. We can consider two cases: i) the discrete breather is weakly localized and ii) the discrete breather is strongly localized. In case i) we are close to the continuous description, and moving breathers are not a surprise. However case ii) is nontrivial. It turns out that up to now case ii) has been reported only for one-dimensional lattices with $V(z) = 0$ (so-called Fermi-Pasta-Ulam systems) [13]. All other systems considered did not show up with moving breathers. So the movability in its strict sense appears to be a quite isolated phenomenon.

Due to the circumstance that time-periodic stationary breathers come in one-parameter families, the excitation of a moving entity starting with an exact stationary breather does not necessarily require changes in the energy. Thus the idea of defining a Peierls-Nabarro potential for the moving entity (in analogy to the problem of moving kinks in lattices) is ill-defined. The high dimensionality of the separatrix which separates stationary objects (perturbed breathers) from possible moving entities is the reason for having an infinite number of possibilities to cross the separatrix with increase, decrease or even no change in energy [14].

2.7 Interaction with Phonons and Electrons

Breathers can strongly scatter phonons and electrons. The phonon scattering problem is in essence similar to the problem of dynamical stability of a breather. Numerical studies revealed that the transmission coefficient for phonons (through a breather) decreases exponentially with increasing wave number [15]. The breather interaction with electrons has been considered within adiabatic approximation, where the lattice vibrations are described classically [16]. Then it is straightforward to show that band electrons are scattered by a breather who acts as a time-dependent (periodic) dipole obstacle. Band edge electrons can be trapped by a breather because band edge states become localized due to the localized character of the corresponding potential mediated by the breather.

3 Conclusion

Discrete breathers are time-periodic localized solutions of classical Hamiltonian lattice equations. Discrete breathers are structurally stable and generic - as opposed to their continuum relatives (e.g. the sG breather). The main reason for this is the existence of a finite upper bound of the linear spectrum of the lattice. Consequently it becomes easy to escape from resonances between multiples of the breather's frequency and the linear spectrum. Discrete breathers can be dynamically stable too. This, together with the fact that discrete breathers come in one-parameter families, makes these objects highly interesting for any physical problem where discreteness is of importance. Discrete breathers appear independently of the lattice dimension - this is a drastic difference as compared to conventional soliton theory. The possibility of local excitation of a lattice whithout subsequent dispersion of the energy pulse makes breathers highly interesting for applications.

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