Optic discrete breathers in Euclidean invariant systems

R.S.MacKay,
Mathematics Institute, University of Warwick,
Coventry CV4 7AL, U.K.

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Abstract

Existence of optic discrete breathers is proved in Euclidean invariant systems with narrow, weakly piezoactive optic band.

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1 Introduction

Discrete breathers (DB) are time-periodic spatially localised vibrations of a network of oscillators (or rotors or spins). Their existence has been proved for Klein-Gordon networks, where each unit has an on-site potential and the units are weakly coupled [MA] (extended in [SM] in ways that we will need here).

On-site potentials, however, are artificial. They model the effects of other degrees of freedom which hold the network together. A good model should include these other degrees of freedom and have no external potential. Thus it would be Euclidean invariant, meaning that the dynamics is equivariant under isometries of real space: if we translate or rotate a possible motion of a crystal or biomolecule we should get another one. Note that we do not require the system to have crystal symmetry; indeed it does not even have to be infinite in extent.

The result of [MA] does not apply to Euclidean invariant systems, for the simple reason that the phonon spectrum Ω includes 0 (isometries), so the non-resonance condition[1] $n\omega_b \notin \Omega$ fails for $n = 0$ for all candidate breather frequencies ω_b. One might think that it is trivial to remove isometries, but there are

[1] Although stated in [MA] only in the special case of the uncoupled limit, it was clear to us that this is a necessary condition for smooth continuability of DB with respect to generic smooth perturbation. Note, however, that in contrast to the uncoupled limit, it is not in general sufficient: there could be a localised Floquet mode with a multipier $+1$.

also phonon frequencies (acoustic modes) within $1/L$ of 0, where L is the system diameter, so standard fixes would not give a result uniform in the system size.

Nonetheless, numerics indicate that discrete breathers can occur in Euclidean invariant systems, e.g. [ST, Pa, FCP, FKT, KBS, KS].

We make a distinction between two types of discrete breather in Euclidean invariant systems: acoustic and optic. Acoustic DB can be viewed as the end result of modulational instability of acoustic phonons, e.g. [SP]. They have frequency near the acoustic phonon band and can have a large width compared with the interatomic spacing. Optic DB can be viewed as oscillation of one degree of freedom (DoF) which is weakly coupled to the rest. In linear theory, such a DoF generates a narrow band of phonon frequencies well separated from 0. The optic DB have frequency near the optic band.

We do not yet have a general proof of existence of acoustic DB, though [Fl] gave one for the special case of pure power FPU chains (details completed by [MS]), and a variational strategy is under investigation for more general FPU chains (Friesecke and MacKay).

Optic DB, on the other hand, have been proved to exist in a number of situations. First, [LSM] proved their existence in diatomic FPU chains with large mass ratio, by solving for the oscillatory motion subject to given mean positions of the heavy masses and then relaxing the resulting energy function of the heavy mass separations. Then [Au2] developed an approach for models with a crystal lattice and exactly linear acoustic modes, coupled linearly to the optic DoF, by solving the linear problem for the acoustic modes given imposed motion of the optic DoF and then solving the resulting problem for the optic DoF. But crystal periodicity and exactly linear acoustic modes and acoustic-optic coupling are strong restrictions.

The present paper provides a much more general proof of existence of optic DB for Euclidean invariant systems. The basic strategy is the same as in [LSM], and has two steps. I applied it to the model of [FCP] during a workshop in Crete in September 1996, and presented the general plan at a workshop in Dresden in April 1997, and at STAMM in Nice in May 1998. Step 1 is to solve for the oscillatory motion subject to given mean positions, and then step 2 is to relax the resulting energy function of the mean positions to a critical point. The second step is the subtle one, because it is here that the Euclidean invariance shows its face. To solve it, I introduced a new norm on the space of configurations of a collection of points in Euclidean space modulo isometries. The solution of this self-contained statics problem has been written up in [Mac]. Thus all we have to do here is to explain step 1 and put the two steps together.

The result has two non-trivial features, however:

1. Although the oscillatory part of the DB decays exponentially in space for many models, it has in general a DC component which decays only like a power law (or not at all in 1D). Aubry called this “piezo-activity” [Au2]. The point is that in general the presence of oscillation changes the mean force between nearby atoms, so the DB induces a static defect, and a static defect in an elastic medium in d dimensions induces a displacement which

behaves like r^{1-d} with respect to distance r from the defect. In the case $d = 1$, the displacement field can be called a kink. The DC kink component of a DB in 1D was already predicted by [KK], re-predicted by [TH] and then [KBS], and proved for diatomic FPU chains with asymmetric potential by [LSM]. The higher dimensional DC distortion was predicted by [KS] and demonstrated by [FKT].

2. In general, the resulting solution is not strictly speaking time-periodic, because a periodic oscillation can induce a net rotation even at zero angular momentum (e.g. [LR]). The DC part of the solution is an equilibrium only up to isometries, so the DB is time-periodic only up to isometry. For large systems, however, the induced rotation rate is very small and can be cancelled by a slight angular momentum.

2 The Models

We consider Euclidean invariant Hamiltonian systems $H(x, p_x, y, p_y)$ with two types of degree of freedom: the "acoustic" DoF x_r and the "optic" DoF y_s, (where r and s are labels), such that if the acoustic DoF are frozen then there are DB for the remaining optic system $H_{x,p_x}(y, p_y)$. By Euclidean invariance we mean that there is an action ϕ of the special Euclidean group $SE(d)$ on the state space, for some dimension d, such that for all $g \in SE(d)$, $H(\phi_g(x, p_x, y, p_y)) = H(x, p_x, y, p_y)$. We will prove that under suitable conditions there are DB for the full system.

For example, the optic DoF y_s might represent the 3D displacement vector along the covalent bond in a diatomic molecule labelled s, and the acoustic DoF x_r the position of the centre of mass of the molecule r in 3D (in this case, r and s run through the same label set). The group action is the obvious one of $SE(3)$: for g a rotation, ϕ_g rotates each of the x_s, p_{x_s}, y_s and p_{y_s} about 0; for g a translation, ϕ_g translates each of the x_s but does nothing to the other coordinates. We suppose that for some reference configuration of the acoustic DoF x, there is a non-degenerate DB for the optic DoF y. This would be the case, for instance, if for frozen x, the y_s are uncoupled 3 DoF oscillators with a non-degenerate equilibrium (depending on the configuration of the neighbouring x_r for example), and a normally non-degenerate family of periodic orbits (e.g. stretches), non-resonant with the linearised motion about equilibrium. By the theory of DB for Klein-Gordon systems as presented in [SM], the DB would also persist if some interaction (but not too much) were turned on between the y_s. The DB would also persist under small changes in the configuration of the frozen acoustic variables x. What counts as small here is really only small changes in the relative positions of nearby x_r, and we will recall from [Mac] a formulation of a suitable norm to quantify this.

As a second type of example, the acoustic variables x_r might represent the positions of heavy atoms, and the optic variables y_s the positions of light atoms relative to certain of the x_r. Imagine the heavy atoms arranged in some graph in

2D or 3D with one light atom near some point of each edge. Protons in hydrogen bonds are a good example of the light atoms. The position of a light atom in 2D can be specified by giving its components along and perpendicular to the edge, with respect to a chosen orientation of the edge. In 3D, one has to use three heavy atom positions to construct a coordinate system for each light atom position. Another situation which fits this scenario is when the heavy atoms form "cages" and there is one light atom near the centre of each cage; then one can specify the light atom's position relative to its cage. The group action is again the obvious one. We suppose that for some reference configuration of the acoustic DoF there is a DB for the optic DoF. This would be the case for example if for frozen x the y_s are uncoupled and each has a non-degenerate equilibrium (depending on the neighbouring x_r) and a normally non-degenerate family of periodic orbits (e.g. vibration along the edge), non-resonant with the linearised motion about equilibrium. The same comments apply as for the first class of examples.

3 The strategy

Periodic orbits of given period T of a Hamiltonian $H : M \to \mathbb{R}$ correspond to critical points of the action functional:

$$S(\gamma) = \int p.dq - Hdt, \tag{1}$$

on the space Γ of period-T loops $\gamma = (q,p) : S^1_T \to M$, where $S^1_T = \mathbb{R}/T\mathbb{Z}$. One could alternatively work with scaled time so that T can be treated as an extra parameter, or to use a variational principle for periodic orbits of given area $A = \int p.dq$ or given energy, or a whole one-parameter family [SM].

Suppose we are given an equilibrium (x_e, y_e) and a non-degenerate DB of period T of the system with acoustic DoF frozen to $x = \bar{x}$, for some $\bar{x}$ "near" x_e, for which y tends to y_e as the distance from the DB increases (the latter condition is not necessary, but is the primary case of interest and is implicit in the definition of DB). As already mentioned, we can continue it to a DB for all nearby $\bar{x}$.

Step 1 is, for each $\bar{x}$ in this set, to continue the DB for x frozen at $\bar{x}$ to a critical point of S on the space $\Gamma_{\bar{x}}$ of loops where x can fluctuate but with mean x fixed to $\bar{x}$. This can be done if the effects of the optic DoF on the acoustic DoF and their back-reaction on the optic DoF are weak in a suitable sense. For example, if the acoustic DoF are heavier by a factor μ then the effect of the optic DoF on them is of order $1/\sqrt{\mu}$. If the acoustic DoF are centre of mass coordinates for molecules then the effect of the optic DoF on them is of order the amplitude of oscillation of the optic DoF. Call the resulting critical value $J(\bar{x})$.

Step 2 is to make J stationary with respect to $\bar{x}$. This is only a statics problem, but it inherits the Euclidean invariance, which makes any equilibrium degenerate. To treat this, we work on the space of configurations $\bar{x}$ modulo isometries, with one of the special ℓ_2 metrics described in [Mac]. These metrics are based on the set of lengths of the edges in a graph connecting the points of $\bar{x}$.

The result is a critical point $\bar{x}$ of J and associated critical loop γ of $S|_{\Gamma_{\bar{x}}}$, thus a critical loop of S on Γ, so a periodic orbit of period T. Its oscillatory part has the spatial localisation properties of a DB of a Klein-Gordon network, because the results of [BM1] or [BM2] apply for exponentially or algebraically decaying coupling respectively, but its DC component has spatial properties characteristic of the solution of the Euclidean invariant statics problem, which in general behaves like r^{1-d}.

4 Discussion

The method can also be used to make multibreathers for Euclidean invariant systems, with any finite number of excited sites. Phase shift degeneracy can be either removed by time-reversal symmetry if present, or handled by forming an effective potential as in [Au1, AMS]. The question arises, however, whether one can make multibreathers with arbitrarily many excited sites, uniformly in the system size. Contrary to my early expectations, a counterexample suggested by [Au2] is correct (proof given in [Mac]). Aubry and I share the view, however, that it is possible there is a class of distributions of breathers for which uniform continuation does hold, and it would be very interesting to identify this class precisely.

As presented, the method works only for weakly piezoactive materials (note that the same is true of [Au2] even though not explicitly admitted there). It is applicable more generally, however, because it is only a question of what reference configuration one perturbs about. For a strongly piezoactive material one has to anticipate a suitable reference state and work near it.

It would be interesting to investigate the stability of these discrete breathers (extending the results of [Au2]), using the techniques of [MSe].

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