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Discrete breathers in anharmonic models with acoustic phonons

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ABSTRACT. – We prove the existence of breathers in a wide family of models consisting of an array of anharmonic molecules coupled by harmonic acoustic phonons. In addition to the usual assumption that the breather frequency and its harmonic do not lie in the phonon bands, an essential hypothesis for this theorem is that the sound velocities in the crystal do not vanish. We are led to distinguish between piezoactive breathers which generates a strain in the crystal which decays at infinity similarly to the electric field of a Coulomb charge, and the nonpiezoactive breathers which generate a strain analogous to the electric field of an electric dipole. A consequence is that the existence proof extends for multibreathers only with a finite number of breathers in the piezoactive case, but for an infinite number and arbitrary configurations in the nonpiezoactive case. In that models, the amplitude of the time dependent harmonics of a single breather decay exponentially with the distance but the static component decays as a power law which is the same as those of a static impurity in the same model. © Elsevier, Paris.

Key words: Breathers, anticontinuous limit, phonons, FPU chains, anharmonic oscillators

RÉSUMÉ. – Nous démontrons l'existence de « breathers » pour une large classe de modèles constitués d'un réseau de molécules anharmoniques couplées par des phonons acoustiques harmoniques. En plus de l'hypothèse usuelle selon laquelle la fréquence des « breathers » ainsi que ses harmoniques ne se situent pas les bandes de phonons, nous imposons

l'hypothèse essentielle à notre résultat, que la vitesse du son ne s'annule pas. Nous sommes conduit à distinguer les « breathers » piézoactifs générant une contrainte dans le cristal s'annulant à l'infini comme le champ électrique d'une charge Coulombienne, de ceux qui ne le sont pas et engendrant une contrainte analogue au champ électrique d'un dipôle.

Une conséquence est que la preuve d'existence s'étend à des « multi-breathers » ne comportant qu'un nombre fini de « breathers » piézoactifs mais un nombre infini et des configurations arbitraires de « breathers » non piézoactifs.

Dans ces modèles, l'amplitude des harmoniques dépendant du temps d'un « breather » simple décroît exponentiellement avec la distance tandis que sa composante statique décroît en loi de puissance de façon similaire à celle d'une impureté statique dans le même modèle.

1. INTRODUCTION

The pioneering work of Sievers and Takeno [1] revealed the existence of time periodic and spatially localized solutions (breathers) in large class of dynamical models (for a review see ref. [2]). Rigorous proofs for their existence were established later [3] for a family of models in arbitrary dimension, which possess a limit called anticontinuous (or anti-integrable [4, 5]) where the model reduces to an array of uncoupled anharmonic oscillators. At this anticontinuous limit, a single breather consists of a single oscillator oscillating while the others are at rest. Under rather weak hypotheses, it was proven that such time reversible solutions could be continued up to a nonzero finite coupling between the oscillators as a consequence of the implicit function theorem. The existence of multibreather states (corresponding to an arbitrary subset of oscillators) oscillating with the same period was also established with the same proof. A series of extensions of these theorems were given later for rotors instead of oscillators, for itinerant electrons coupled with anharmonic oscillators [6], for nonhamiltonian systems with dissipation and more generally for coupled multicomponent oscillators [7, 8].

At the anticontinuous limit of the hamiltonian systems with breathers where these proofs hold, the phonon dispersion corresponding to the linearized fluctuations around the ground-state consists of a perfectly flat optical branch. In models involving acoustic phonons for example the FPU

chains, such an anticontinuous limit cannot be defined. A method which works successfully for numerical calculations [9] consists in starting from the anticontinuous limit of a variation of these models where an extra substrate potential is introduced. Its breather solutions can be continued when varying the model parameters along an appropriate path, till the initial model is recovered. However, although this breather continuation can be observed numerically, the mathematical proof that this continuation is possible all along the path, seems to be a delicate task.

Some attempts to prove the existence of breathers to models with acoustic phonons, were made by introducing new anticontinuous limits at which the existence of breathers is trivial, can be defined and used for continuation. In [10], 1d models with two types of atoms with different masses are considered. An anticontinuous limit is obtained when the mass ratio between light and heavy atoms goes to zero. At this limit, the heavy atoms are static and do not respond to the vibrations of the light atoms, thus playing the role of a substrate potential. There are breather solutions which can be continued when the mass ratio varies up to some non vanishing value. This method was claimed to be extendable to higher dimension [11].

The essential technical difficulty (which has a physical origin) for extending the proof of the breather existence in systems with acoustic phonons is that in case a breather would exist with some frequency ω_b in a system, and although it does not couple to the global translation modes, the breather harmonic 0 is always almost resonant with the acoustic phonons in the long wave length limit. Thus the crucial point is to control how this coupling vanishes and to show that it is harmless for the existence of breathers.

Section (2) of the paper defines the class of models on which we work and the notation. In section (3), we introduce the concept of piezoactivity of an optical mode and distinguish between piezoactive and non piezoactive optical modes. The next section (4) discusses the structural stability of periodic orbits in anharmonic oscillators with a finite number of components. In section (5), we describe some specific models which belong to the general class of models and illustrate the concept of piezoactivity. The next section (6) presents a proof of existence of piezoactive breathers or finite multibreathers and the next section (7) presents a specific proof for nonpiezoactive breathers which also holds for infinite multibreathers. In section (8), we suggest extension of these results for nontime reversible breathers and especially rotobreathers. We also suggest extensions to random network. We discuss briefly how the last limitation of our model, which is the harmonicity of the acoustic phonons could be overcome. Section (9)

discusses the breather extension for the dynamical part and the linear stability of the single breathers. Finally, we conclude in the last section (10) by some brief suggestions of their relevance for some problems of physics and biology.

2. DESCRIPTION OF THE CLASS OF MODELS

We consider here different types of models which are broad d-dimensional extensions of the 1d model considered in [12] where acoustic breathers were already found numerically. These models consist of arrays of anharmonic molecules (e.g. two atoms coupled by an anharmonic potential). These molecules are coupled one with each other by harmonic potentials in order to form a d-dimensional lattice with acoustic and optical phonons. The limit we call anticontinuous is obtained when this coupling is zero. This class of models does not include FPU chains for which specific proofs are needed [15].

The basic principle of our approach is to eliminate the acoustic variables which can be made explicitly because they are assumed to be *harmonic*. This elimination results in an effective (retarded) coupling between the variables of the anharmonic molecules. Although we get long range interactions between the oscillators, the conditions for the applicability of the implicit function theorem to this effective model, are preserved if one chooses appropriate norms.

Although these models do not yet describe the fully general case where all the crystal interactions should be assumed anharmonic, they clearly demonstrate how breathers survive in the presence of acoustic phonons.

2.1. The Hamiltonian

The crystal is in a d dimensional space which contains in each unit cell $\mathbf{n} \in \mathcal{Z}^d$, an anharmonic molecule which we choose for simplicity to be diatomic, and N_c other atoms ($p = 1, \ldots, N_c$).

The mass of each molecule in the unit cell $\mathbf{n}$ is M_0 and $\mathbf{x}_{\mathbf{n},0}$ is the vector describing the displacement of its center of mass referred to its position in the crystal in equilibrium at rest. The displacements of the other N_c atoms p with mass M_p in the unit cell $\mathbf{n}$ also referred from their positions at rest are denoted $\mathbf{x}_{\mathbf{n},p} = \{x_{\mathbf{n},p,\alpha}\}$ (α labels the d space directions). The internal coordinate of molecule $\mathbf{n}$, in the framework of its center of mass, is

described by the d-dimension vector $\mathbf{y_n} = \{y_{\mathbf{n},\alpha}\}$ [1]. Thus, when the crystal is in equilibrium at rest, all the coordinates are zero.

More generally, vector $\mathbf{y_n}$represents the anharmonic optical variables (*i.e.* which are unchanged by crystal translations) in the unit cell of the crystal and has not necessarily the dimension d. Nevertheless, we shall continue to assume in order to fix the ideas that it has dimension d.

With $\mathbf{X} = \{x_{\mathbf{n},p,\alpha}\}$ denoting the global vector describing all the components of the displacements of the atoms and molecules, and $\mathbf{Y} = \{y_{\mathbf{n},\alpha}\}$, the vector for the internal coordinates of the molecules, the Hamiltonian of this system has the form

$$\mathbf{H} = \mathbf{H}_{elst} + \mathbf{H}_{AC} + k\mathbf{Y}^t.\mathbf{P}.\mathbf{X} + k'\mathbf{W}(\mathbf{Y}) \tag{1}$$

where

$$\mathbf{H}_{elst} = \sum_{\mathbf{n},p} \frac{1}{2} M_p \dot{\mathbf{x}}_{\mathbf{n},p}^2 + \frac{1}{2}\mathbf{X}^t.\mathbf{N}.\mathbf{X} \tag{2}$$

is a standard harmonic Hamiltonian of some d dimensional perfect crystal with $d(n+1)$ variables per unit cell and the positive elasticity matrix $\mathbf{N}$. The crystal energy is assumed to be invariant by any global spatial translation in any of the d directions. Then, we have $\mathbf{N}.\mathbf{1}_\alpha = \mathbf{0}$ for each unit translation in the space direction α. $((\mathbf{1}_\alpha)_{\mathbf{n},p,\beta} = \delta_{\alpha,\beta})$. Zero is a degenerate eigenvalue of $\mathbf{N}$ with order of degeneracy d. Thus, this matrix is not strictly positive and is not invertible.

$\mathbf{H}_{AC}$ is the Hamiltonian which describes the anharmonic internal vibrations of the molecules

$$\mathbf{H}_{AC} = \sum_{\mathbf{n}} \left(\frac{1}{2} m \dot{\mathbf{y}}_{\mathbf{n}}^2 + V(\mathbf{y_n}) \right) \tag{3}$$

It just consists of uncoupled oscillators with mass m and anharmonic d dimensional C^2 potential $V(\mathbf{y})$ (that is twice differentiable with continuous derivatives). This potential is defined as resulting from the interaction of the considered molecule with the neighboring atoms and molecules *fixed at their rest position* for the crystal in a fixed orientation. In general, this potential $V(\mathbf{y_n})$ has the local symmetry of the crystal which is not the spherical symmetry of the potential for a completely free molecule.

[1] For example, if molecule $\mathbf{n}$ consists of two atoms with coordinates $\mathbf{u_n}$ and $\mathbf{v_n}$ and masses m_1 and m_2 respectively, the coordinate of its center of mass is $\mathbf{x}_{\mathbf{n},0} = (m_1\mathbf{u_n} + m_2\mathbf{v_n})/(m_1 + m_2)$ and its internal coordinate is $\mathbf{y_n} = \mathbf{v_n} - \mathbf{u_n}$.

It will not cost more work in the existence proof if hamiltonian (1) also includes a direct coupling between the internal coordinates of the molecules in neighboring cells $< \mathbf{n}, \mathbf{m} >$ described by the C^2 potential

$$\mathbf{W}(\mathbf{Y}) = \sum_{<\mathbf{n},\mathbf{m}>} W_{\mathbf{n}-\mathbf{m}}(\mathbf{y}_\mathbf{n}\mathbf{y}_\mathbf{m}) \tag{4}$$

with amplitude k' and which could be anharmonic or not.

The other interactions between these molecules and the remainder of the system are treated harmonically. The coupling between the internal coordinates of the molecules and the displacements of the atoms and molecules from their rest positions is described by a matrix $\mathbf{P} = \{P_{(\mathbf{n},\alpha),(\mathbf{m},r,\beta)}\}$. The amplitude of this coupling is controlled by parameter k. The periodicity of the crystal also implies that each matrix element $P_{(\mathbf{n},\alpha),(\mathbf{m},r,\beta)}$ only depends on the difference $\mathbf{n} - \mathbf{m}$ (and on the intracell indices (α) and (r,β). The coupling matrix $\mathbf{P}$ is also invariant by a global translation of the crystal which implies $\mathbf{P}.\mathbf{1}_\alpha = \mathbf{0}$ for all the directions α.

The dynamical equations of this model can be written explicitly as

$$M_p\ddot{x}_{\mathbf{n},p,\alpha} + \sum_{\mathbf{m},q,\beta} N_{(\mathbf{n},p,\alpha),(\mathbf{m},q,\beta)}.x_{\mathbf{m},q,\beta} + k\sum_{\mathbf{m},\beta} P_{(\mathbf{m},\beta),(\mathbf{n},p,\alpha)}.y_{\mathbf{m},\beta} = 0 \tag{5}$$

$$m\ddot{y}_{\mathbf{n},\alpha} + \frac{\partial V(\mathbf{y}_\mathbf{n})}{\partial y_{\mathbf{n},\alpha}} + k\sum_{\mathbf{m},p,\beta} P_{(\mathbf{n},\alpha),(\mathbf{m},p,\beta)}.x_{\mathbf{m},p,\beta} + k'\frac{\partial \mathbf{W}(\mathbf{Y})}{\partial y_{\mathbf{n},\alpha}} = 0 \tag{6}$$

where $\mathbf{M}$ is the diagonal matrix of the atomic and molecular masses M_p.

When $k = 0$, the molecular modes are uncoupled to the harmonic phonons and then the existence of breathers can be proved as before for purely optical breathers [3]. The anticontinuous limit of this model is obtained when $k = k' = 0$. Then, it consists of a standard crystal decoupled from independent anharmonic oscillators.

2.2. Optical and acoustic phonons

We have to make some hypotheses on the model which actually will mean that we just consider a physically realistic crystal. Equation

$$M_p\ddot{x}_{\mathbf{n},p,\alpha} + \sum_{\mathbf{m},r,\beta} N_{(\mathbf{n},p,\alpha),(\mathbf{m},r,\beta)}.x_{\mathbf{m},r,\beta} = 0 \tag{7}$$

determines the phonon spectrum of the uncoupled crystal at $k = k' = 0$. The periodicity of the crystal implies that each matrix element $N_{(\mathbf{n},p,\alpha),(\mathbf{m},r,\beta)}$ only depends on the difference $\mathbf{n} - \mathbf{m}$ (and on the intracell indices (p,α) and (r,β)) (as well as $P_{(\mathbf{n},\alpha),(\mathbf{m},r,\beta)}$).

The phonon spectrum can be obtained using the standard space time Fourier transform

$$x_{p,\alpha}(\mathbf{q}) = \sum_{\mathbf{m}} x_{\mathbf{m},p,\alpha} e^{i\mathbf{q}\mathbf{m}} \qquad \text{and} \qquad y_{\alpha}(\mathbf{q}) = \sum_{\mathbf{m}} y_{\mathbf{m},\alpha} e^{i\mathbf{q}\mathbf{m}} \tag{8}$$

where $\mathbf{q}$ is a d dimension vector and $|q_\alpha| \leq \pi$ for all components α which defines the standard Brillouin zone BZ of a cubic lattice. We define the coefficients of the finite $(n+1)d \times (n+1)d$ matrix $\mathbf{N}(\mathbf{q})$ and $d \times (n+1)d$ matrix $\mathbf{P}(\mathbf{q})$ as

$$N_{(p,\alpha),(r,\beta)}(\mathbf{q}) = \sum_{\mathbf{m}} e^{-i\mathbf{q}.\mathbf{m}} . N_{(\mathbf{n},p,\alpha),(\mathbf{n}+\mathbf{m},r,\beta)} \tag{9}$$

$$P_{(\alpha),(r,\beta)}(\mathbf{q}) = \sum_{\mathbf{m}} e^{-i\mathbf{q}.\mathbf{m}} . P_{(\mathbf{n},\alpha),(\mathbf{n}+\mathbf{m},r,\beta)} \tag{10}$$

Then, it comes out after time Fourier transform that

$$-\omega^2(\mathbf{q}) M_p x_{p,\alpha}(\mathbf{q}) + \sum_{r,\beta} N_{(p,\alpha),(r,\beta)}(\mathbf{q}) . x_{r,\beta}(\mathbf{q}) = 0 \tag{11}$$

determines $\omega^2(\mathbf{q})$ as an eigenvalue of the $d(n+1) \times d(n+1)$ matrix $\mathbf{M}^{-1}.\mathbf{N}(\mathbf{q})$ and the corresponding eigenmode. There are $d(n+1)$ phonon branches $\omega_\nu(\mathbf{q})$. Since the translation invariance of the crystal energy in the d directions, implies that $\mathbf{N}$ has d degenerate eigenvectors for the eigenvalue 0, there are d branches of (acoustic) phonons $\omega_{ac}(\mathbf{q})$ which vanishes at $\mathbf{q} = 0$ and are assumed to be strictly positive for $\mathbf{q} \neq 0$ (that is the crystal is stable). There are also nd branches of optical phonons $\omega_{opt}(\mathbf{q})$ which are strictly positive for all $\mathbf{q}$. Thus, the finite matrices $\mathbf{N}(\mathbf{q})$ are strictly positive and invertible for $\mathbf{q} \neq 0$. However, matrix $\mathbf{N}(\mathbf{0})$ is not invertible and consequently the whole matrix $\mathbf{N}$ is not invertible as well. This noninvertibility makes *a priori* the continuation of breathers questionable when there are acoustic phonons. Actually, this apparent difficulty can be overcome provided we make assumptions which are nothing but characteristics of physically realistic models.

To prove breather continuation, we need first to assume that matrices $\mathbf{N}$ and $\mathbf{P}$ involve interactions between the atoms and molecules which are not (too much) long range. This condition is precisely formulated by assuming that matrices $\mathbf{N}(\mathbf{q})$ and $\mathbf{P}(\mathbf{q})$, are C^2 functions of the wavevector $\mathbf{q}$. As a result, the phonon frequency squares are C^2. The phonon frequencies $\omega_\nu(\mathbf{q})$ are also C^2 except at $\mathbf{q} = \mathbf{0}$ for the d acoustic phonon branches labeled ac, $\omega_{ac}(\mathbf{q})$.

For those branches, we have $\omega_{ac}(\mathbf{0}) = 0$ and $\omega_{ac}^2(\mathbf{q})$ can be expanded for small $|\mathbf{q}|$ as $\omega_{ac}^2(\mathbf{q}) \simeq < \mathbf{q}|\mathbf{\Omega}_{ac}|\mathbf{q} >$ where $\mathbf{\Omega}_{ac}$ is $d \times d$ matrix which determines the sound velocities in the crystal. They are defined as the slopes of the acoustic phonon branches in the different eigendirections of the d matrices $\mathbf{\Omega}_{ac}$ that is the squareroots of their eigenvalues [2]. In a real crystal, the sound velocities are generally not zero so that $\omega_{ac}(\mathbf{q})$ is not C^2 at $\mathbf{q} = \mathbf{0}$.

As well as those of matrix $\mathbf{M}^{-1}.\mathbf{N}(\mathbf{q})$, there are d eigenvalues $\lambda_{ac}(\mathbf{q})$ for matrix $\mathbf{N}(\mathbf{q})$ which vanishes at $\mathbf{q} = \mathbf{0}$ and can be expanded for small $\mathbf{q}$ as

$$\lambda_{ac}(\mathbf{q}) \simeq < \mathbf{q}|\mathbf{C}_{ac}|\mathbf{q} > \tag{12}$$

The eigenvalues of $\mathbf{C}_{ac}$ are strictly positive. Using the fact that the mass matrix $\mathbf{M}$ is strictly positive, it is straightforward to show that this property is equivalent to say that the sound velocities of the crystal do not vanish.

When k and k' are not zero, the phonon spectrum corresponding to the linearized small oscillation is modified by the coupling with the internal extra molecular modes. The sound velocities turn out to be reduced by the coupling. The stability of the crystal at equilibrium requires that the phonon frequency squares and especially the acoustic ones, do not become negative. This condition is fulfilled when k and k' are not too large which is the regime we are interested in.

3. PIEZOACTIVE AND NONPIEZOACTIVE MODES

Our approach for studying the existence of breathers is based on the elimination of the harmonic variables $\mathbf{X}$. It turns out that the anharmonic coordinates might be coupled to the acoustic phonons in two ways

[2] Taking into account the fact that for $\mathbf{y} = \mathbf{0}$, the crystal energy is unchanged by any global crystal rotation, there are only $d(d-1)/2$ different sound velocities in the most general case without special symmetries.

depending on the symmetries of the model. We are led to distinguish between piezoactive and non piezoactive coordinates.

For the elimination of $\mathbf{X}$, only the static part will cause problem. Thus we consider preliminarily the static problem where the internal coordinates are fixed to arbitrary values $\mathbf{Y}$. Then, $\mathbf{X}$ is determined by minimizing the part of the energy

$$\Phi(\mathbf{X},\mathbf{Y}) = \frac{1}{2}.\mathbf{X}^t.\mathbf{N}.\mathbf{X} + k\mathbf{Y}^t.\mathbf{P}.\mathbf{X} \tag{13}$$

in (1) which depends on $\mathbf{X}$. It comes out $\mathbf{X} = -k\mathbf{N}^{-1}.\mathbf{P}^t.\mathbf{Y}$ and the minimum of this energy is

$$\Phi_M(\mathbf{Y}) = -\frac{k^2}{2}.\mathbf{Y}^t.\mathbf{P}.\mathbf{N}^{-1}.\mathbf{P}^t.\mathbf{Y} \tag{14}$$

Actually, $\mathbf{N}$ is in principle not invertible and we have to give a precise definition to the products

$$\mathbf{R}_0 = \mathbf{N}^{-1}.\mathbf{P}^t \qquad \text{and} \qquad \mathbf{S}_0 = \mathbf{P}.\mathbf{N}^{-1}.\mathbf{P}^t \tag{15}$$

In the Fourier representation (8),we have for $\mathbf{q} \neq \mathbf{0}$,

$$\mathbf{x}(\mathbf{q}) = -k\mathbf{N}^{-1}(\mathbf{q}).\mathbf{P}^t(\mathbf{q}).\mathbf{y}(\mathbf{q}) \tag{16}$$

and $\Phi_M(\mathbf{Y}) = 1/(2\pi)^d \int \Phi_{\mathbf{q}} d\mathbf{q}$ with

$$\Phi_{\mathbf{q}} = -\frac{1}{2}\mathbf{y}^t(\mathbf{q}).\mathbf{P}(\mathbf{q}).\mathbf{N}^{-1}(\mathbf{q}).\mathbf{P}^t(\mathbf{q}).\mathbf{y}(\mathbf{q}) \tag{17}$$

The $(n+1)d \times d$ matrix $\mathbf{R}_0(\mathbf{q}) = \mathbf{N}^{-1}(\mathbf{q}).\mathbf{P}^t(\mathbf{q})$ can be expanded as

$$\mathbf{R}_0(\mathbf{q}) = \sum_\nu |\mathbf{V}_\nu(\mathbf{q}) > \frac{1}{\lambda_\nu(\mathbf{q})} < \mathbf{V}_\nu(\mathbf{q})|.\mathbf{P}^t(\mathbf{q}) \tag{18}$$

where $|\mathbf{V}_\nu(\mathbf{q}) >$ are the $d(n+1)$ normalized eigenvectors of $\mathbf{N}(\mathbf{q})$ with strictly positive eigenvalues $\lambda_\nu(\mathbf{q})$.

When $\mathbf{q} \to \mathbf{0}$, there are d eigenvalues labeled $\lambda_{ac}(\mathbf{q})$ which go to zero while the corresponding eigenvectors $|\mathbf{V}_{ac}(\mathbf{q}) >= \{V_{p,\alpha,ac}(\mathbf{q})\}$ become global crystal translations combinations of the unit vectors $\mathbf{1}_\alpha$ The translational invariance of the energy of the crystal implies that vector $< \mathbf{U}_{ac}(\mathbf{q})| =< \mathbf{V}_{ac}(\mathbf{q})|\mathbf{P}^t(\mathbf{q})$ with $U_{ac,\alpha}(\mathbf{q}) = \sum_{r,\beta} P_{(\alpha),(r,\beta)}(\mathbf{q})$

$V_{r,\beta,ac}(\mathbf{q})$ goes to zero. Since we have $\mathbf{U}_{ac}(\mathbf{q}) = \mathbf{U}^*_{ac}(-\mathbf{q})$, it can be expanded for small $|\mathbf{q}|$ as

$$U_{ac,\alpha}(\mathbf{q}) \simeq i\mathbf{B}_{ac,\alpha}|\mathbf{q}> + <\mathbf{q}|\mathbf{A}_{ac,\alpha}|\mathbf{q}> \tag{19}$$

Actually, $\mathbf{A} = \{\mathbf{A}_{ac}\} = \{\mathbf{A}_{ac,\alpha}\} = \{A_{(ac,\alpha),(\beta,\gamma)}\}$, $\mathbf{B} = \{\mathbf{B}_{ac}\} = \{\mathbf{B}_{ac,\alpha}\} = \{B_{(ac,\alpha),\beta}\}$ and $\mathbf{C} = \{\mathbf{C}_{ac}\} = \{C_{(ac),(\beta,\gamma)}\}$ are real tensors where the first group of indices deals with the label of the acoustic branch ac and the space direction α while the second group deals with d the components of $\mathbf{q}$. For simplicity in the notations used in the next, we implicitly assume that $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are matrices either with respect to the first group of indices or with the second group.

There are two possible situations which can be met in models, depending whether $\mathbf{B}$ vanishes (for all components) or not. We distinguish between the case where $\mathbf{B}$ does not vanish called "piezoactive" from the other case where it does.

3.1. Case with a piezoactive coupling

There are components of $\mathbf{B}$ which do not vanish. It is reasonable to expect this situation for the most realistic models of crystals since a local vibration of a molecule tends to increase its effective volume and develops a strain in the crystal around it.

As a result, when $\mathbf{q} \to \mathbf{0}$, operator $\mathbf{R}_0(\mathbf{q})$ in eq.18, diverges as

$$(\mathbf{R}_0(\mathbf{q}))_{\alpha,\beta} \simeq \frac{i}{|\mathbf{q}|} \sum_{ac} |V_{p,\alpha,ac}(\mathbf{0})> . \frac{1}{<\hat{\mathbf{q}}|\mathbf{C}_{ac}|\hat{\mathbf{q}}>} .(\mathbf{B}_{ac,\beta}|\hat{\mathbf{q}}>) \tag{20}$$

where $\mathbf{q} = |\mathbf{q}|.\hat{\mathbf{q}}$ defines the unitary vector $\hat{\mathbf{q}}$.

For a distortion of the anharmonic coordinates $\mathbf{y_n} = \cos < \mathbf{n}|\mathbf{q} > \mathbf{u}$ in the direction $\mathbf{u}$, we get the distortion of coordinates $\mathbf{x_n} = \sin < \mathbf{n}|\mathbf{q} > .\mathbf{R}_0(\mathbf{q}).\mathbf{u}$. When $\mathbf{q} \to \mathbf{0}$, it comes that

$$\mathbf{x_n} \simeq -k < \mathbf{n}|\hat{\mathbf{q}} > \sum_{ac} \frac{(\mathbf{B}_{ac}|\hat{\mathbf{q}}>)^t.|\mathbf{u}>}{<\hat{\mathbf{q}}|\mathbf{C}_{ac}|\hat{\mathbf{q}}>} |\mathbf{V}_{ac}(\mathbf{0})> \tag{21}$$

Locally, this distortion is collinear to a crystal translation but is unbounded and diverges linearly as $< \mathbf{n}|\mathbf{q} >$ in the direction of $\hat{\mathbf{q}}$. The

effect of this distortion is to stretch or to shear uniformly the crystal which change the macroscopic size and the shape of the crystal. We say that the internal mode of the molecule is piezoactive [3].

The coefficients $= \{R_{(\mathbf{n},p,\alpha),(\mathbf{m},\beta)}\}$ of matrix $\mathbf{R}_0$ are the Fourier transform of those of $\mathbf{R}_0(\mathbf{q})$

$$R_{(\mathbf{n},p,\alpha),(\mathbf{m},\beta)} = \frac{1}{(2\pi)^d} \int_{BZ} e^{i\mathbf{q}.(\mathbf{m}-\mathbf{n})} (\mathbf{R}_0(\mathbf{q}))_{(p,\alpha),\beta} \, d\mathbf{q} \qquad (22)$$

It can be proven that although the singularity (20) at $\mathbf{q} = \mathbf{0}$, this integral (22) can be defined even in one dimension ($d = 1$). However, because of this singularity at $\mathbf{q} = \mathbf{0}$, the coefficients of $\mathbf{R}_0 = \{R_{(\mathbf{n},p,\alpha),(\mathbf{m},\beta)}\}$ depends on $\mathbf{n} - \mathbf{m}$ in a similar way as those of the electric field created by a Coulomb charge at the origin in a d dimensional space.

A local distortion of a single molecule at site $\mathbf{0}$ in the crystal represented by $\mathbf{y}_0 \neq \mathbf{0}$ and $\mathbf{y}_\mathbf{i} = \mathbf{0}$ for $\mathbf{i} \neq \mathbf{0}$, induces a crystal distortion $x_{\mathbf{n},p,\alpha} = -k \sum_\beta R_{(\mathbf{n},p,\alpha),(\mathbf{0},\beta)} y_{\mathbf{0},\beta}$ at infinity which only decays to zero at $d \geq 2$ and goes to a constant in 1 dimension. This is the expected behavior of the distortion induced by an impurity (atomic substitution of an atom by another one with a different size) in a crystal.

Although the matrix $\mathbf{R}_0(\mathbf{q})$ is unbounded, the matrix $\mathbf{S}_0(\mathbf{q}) = \mathbf{P}(\mathbf{q}).\mathbf{N}^{-1}(\mathbf{q}).\mathbf{P}^t(\mathbf{q})$ involved in the energy is bounded for all $\mathbf{q}$ and can be expanded for $\mathbf{q} \to \mathbf{0}$ as

$$\mathbf{S}_0(\mathbf{q}) \simeq -\sum_{ac} (\mathbf{B}_{ac}|\hat{\mathbf{q}}>)^t . \frac{1}{<\hat{\mathbf{q}}|\mathbf{C}_{ac}|\hat{\mathbf{q}}>} . (\mathbf{B}_{ac}|\hat{\mathbf{q}}>) \qquad (23)$$

However, the limit of this operator for $\mathbf{q} \to \mathbf{0}$ is generally not well defined because it depends generally on the direction $\hat{\mathbf{q}}$ in which the limit is taken. Nevertheless, this result implies that the spectrum of operator $\mathbf{S}_0$ considered in the Hilbert space of square summable vectors, is the union of the spectra of $\mathbf{S}_0(\mathbf{q})$, and thus is bounded. As a result, this linear operator

[3] In this present model, and if the molecule bears an electric dipole, this condition generally implies piezoelectricity for the whole crystal. However, in more complex models, we could have other anharmonic modes in the same unit cell which could cancel by symmetry any piezoelectric effect.

$\mathbf{S}_0$ obtained by inverse Fourier transform as in (22), is bounded for the l^2 norm and maps the space of square summable vectors $\mathbf{Y}$ onto itself [4].

The one dimensional case is peculiar because there are only two opposite directions for the unit wavevector $\hat{\mathbf{q}}$. As a result $\mathbf{S}_0(\mathbf{q})$ is continuous at $\mathbf{q} = \mathbf{0}$ which implies that the Fourier series which determines

$$(\mathbf{S}_0(\mathbf{q}))_{\alpha,\beta} = \sum_{\mathbf{m}} S_{(\mathbf{n},\alpha),(\mathbf{n}+\mathbf{m},\beta)} e^{i\mathbf{q}.\mathbf{m}}$$

is absolutely convergent and consequently the sum $\sum_{\mathbf{m}} |S_{(\mathbf{n},\alpha),(\mathbf{n}+\mathbf{m},\beta)}| < \infty$ is convergent. Then, $\mathbf{S}_0$ considered with the standard supremum norm is bounded. It maps the Banach space of vectors $\mathbf{y}$ considered with the standard supremum norm onto itself.

In contrast, in $d \geq 2$ dimensions, $\mathbf{S}_0(\mathbf{q})$ is generally not a continuous function of $\mathbf{q}$ so that the Fourier series (24) cannot be absolutely convergent. We have $\sum_{\mathbf{m}} |S_{(\mathbf{n},\alpha),(\mathbf{n}+\mathbf{m},\beta)}| = \infty$ which implies that $\mathbf{S}_0$ considered with the standard supremum norm is not bounded. $\mathbf{S}_0$ generally does not map the Banach space of vectors $\mathbf{y}$ considered with the standard supremum norm onto itself.

3.2. Case without piezoactive coupling

This situation is less general than the previous one but often occurs in simplified models which have symmetries which force the linear part $\mathbf{B}$ to vanish. Then, for $\mathbf{q} \to \mathbf{0}$

$$\mathbf{R}_0(\mathbf{q}) \simeq \sum_{ac} \frac{< \hat{\mathbf{q}}|\mathbf{A}_{ac}|\hat{\mathbf{q}} >}{< \hat{\mathbf{q}}|\mathbf{C}_{ac}|\hat{\mathbf{q}} >} |\mathbf{V}_{ac} > \tag{25}$$

$\mathbf{R}_0(\mathbf{q})$ is bounded but is generally not continuous at $\mathbf{q} = \mathbf{0}$ (in more than 1 dimension). Then, operator $\mathbf{N}^{-1}.\mathbf{P}^t$ can be defined by its coefficients $R_{(\mathbf{n},p,\alpha),(\mathbf{m},\beta)}$ of $\mathbf{N}^{-1}.\mathbf{P}^t$ which are obtained by inverse Fourier transform of those of $\mathbf{R}_0(\mathbf{q})$. Since $\mathbf{R}_0(\mathbf{q})$ is not continuous, the series $\sum_{\mathbf{m}} |R_{(\mathbf{n},p,\alpha),(\mathbf{n}+\mathbf{m},\beta)}|$ of the absolute values of its Fourier coefficients is divergent, that is the Fourier series cannot be absolutely convergent. The crystal distortion $\mathbf{x}_\mathbf{n}$ induced by a local distortion is bounded but decay slowly as a power function of the distance $\mathbf{n}$ which depends on the crystal and its dimensionality. Although it is more complex, it is similar to the electric field generated by an electric dipole.

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[4] The l^2 norm of vector $\mathbf{Y}$ is $\|\mathbf{Y}\|_2 = \sqrt{\sum_{i,\alpha} |y_{i,\alpha}|^2}$ and its supremum norm is $\|\mathbf{Y}\|_s = \sup_{i,\alpha} |y_{i,\alpha}|$. The l^2 (resp. supremum) norm of an operator $\mathbf{S}_0$ is $\|\mathbf{S}_0\| = \sup_{\mathbf{Y}} \|\mathbf{S}_0.\mathbf{Y}\|/\|\mathbf{Y}\|$ where $\|.\|$ is the l^2 (resp. supremum) vector norm.

Nevertheless, in this case, the energy coupling between the internal coordinates of the molecules and the acoustic variables at $\mathbf{q} = \mathbf{0}$ vanishes. Matrix $\mathbf{S}_0(\mathbf{q})$ can be expanded for $\mathbf{q} \to \mathbf{0}$ as

$$\mathbf{S}_0(\mathbf{q}) \simeq |\mathbf{q}|^2 \sum_{ac} (< \hat{\mathbf{q}}|\mathbf{A}_{ac}|\hat{\mathbf{q}} >)^t . \frac{1}{< \hat{\mathbf{q}}|\mathbf{C}_{ac}|\hat{\mathbf{q}} >} . < \hat{\mathbf{q}}|\mathbf{A}_{ac}|\hat{\mathbf{q}} > \qquad (26)$$

It vanishes at $\mathbf{q} = \mathbf{0}$ and is twice differentiable but with discontinuous second derivatives at $\mathbf{q} = \mathbf{0}$.

In any case, $\mathbf{S}_0(\mathbf{q})$ is a C^0 function of $\mathbf{q}$ which implies that the linear operator $\mathbf{S}_0$ considered with the standard supremum norm is now bounded. It maps the Banach space of vectors $\mathbf{y}$ considered with the standard supremum norm onto itself. It is also bounded as before for the l^2 norm.

4. STRUCTURALLY STABLE PERIODIC ORBITS AT THE ANTICONTINUOUS LIMIT

We also need to make hypotheses on the single d dimensional oscillator corresponding to a noninteracting molecule, in order to have breather solutions which could be continued from the anticontinuous limit $k = k' = 0$. At this limit, the single d dimensional oscillator with dynamical equation

$$m\ddot{y}_\alpha + \frac{\partial V(\mathbf{y})}{\partial y_\alpha} = 0 \qquad (27)$$

is not necessarily an integrable system for $d \geq 2$. It may exhibit (as usual) periodic, quasiperiodic and chaotic solutions. Nevertheless, there are often families of time reversible and time periodic solutions with a continuum of frequencies ω_b [5]. Considering small amplitude oscillation around a time periodic solution $\mathbf{y}(t)$, eq. 27 can be linearized as

$$m\ddot{\epsilon}_\alpha + \sum_\beta V_{\alpha,\beta}(t)\epsilon_\beta = 0 \qquad (28)$$

[5] For example, for $d = 2$, the existence of such solutions may be proven with the former breather existence theorem [3]. Let $\mathbf{y} = (y_1, y_2)$, and assume that $V(\mathbf{y})$ can be written with the form $V(\mathbf{y}) = \mathcal{V}(y_1) + \mathcal{V}(y_2) + C\mathcal{W}(y_1 - y_2)$ where $\mathcal{V}(y)$ and $\mathcal{W}(z)$ are anharmonic potentials. For $C = 0$, this two site model has time periodic solutions which generally can be continued when C is not too large.

where $\mathbf{V} = \{V_{\alpha,\beta}(t)\}$ is a time dependent $d \times d$ matrix with

$$V_{\alpha,\beta}(t) = \frac{\partial^2 V(\mathbf{y}(t))}{\partial y_\alpha \partial y_\beta} \tag{29}$$

For the solution of the oscillator at rest $\mathbf{y}(t) = \mathbf{0}$, this matrix does not depend on time and its d eigenvalues $m\omega_\mu^2 \neq 0$ are the local eigenfrequencies of the molecule.

4.1. Condition of nonresonance

We assume that equation (27) has time periodic and time reversible orbits $\mathbf{y}(t)$ with period $t_b = 2\pi/\omega_b$ (*i.e* which fulfill $\mathbf{y}(t) = \mathbf{y}(t + t_b)$ and $\mathbf{y}(t) = \mathbf{y}(-t)$). In addition, their frequencies should not be "resonant" with the phonon bands that is

• For any integer $p \neq 0$, $p\omega_b$ is not equal to any $\omega_\nu(\mathbf{q})$ for any wavevector $\mathbf{q}$ and phonon branch ν determined by eq. 11.

• For any integer p, $p\omega_b$ is not equal to any of the rest frequencies of the molecule ω_μ.

We also need to assume that the periodic orbits of the individual oscillators, we shall consider are "structurally stable" which means that when the hamiltonian is perturbed by a smooth perturbation term, each orbit is smoothly perturbed but persists with the same period. In the $d = 1$ case [3], this property was expressed in the action angle representation by the condition $d\omega(I)/dI \neq 0$. When, $d \geq 2$, we cannot define an extended action angle representation unless the model is integrable as a consequence of a Liouville theorem [14], but this is an exceptional situation.

It is then convenient to express this property of structural stability through the spectral properties of the linear derivative operator $\{\eta_\alpha\} = \partial T.\{\epsilon_\alpha\}$ defined as

$$\eta_\alpha = m\ddot{\epsilon}_\alpha + \sum_\beta V_{\alpha,\beta}(t)\epsilon_\beta \tag{30}$$

The periodic orbit $\mathbf{y}(t)$ with period t_b is structurally stable if ∂T is invertible for the L^2 topology in the space of time periodic and time reversible solutions $\{\epsilon_\alpha(t)\}$ with the period t_b. Since the number d of components of ϵ_α is finite, the spectrum of this d dimensional Sturm-Liouville operator ∂T, is discrete and consists of isolated eigenvalues with possible finite degeneracy only [13]. Then, the structural stability condition is simply that ∂T has no eigenvalue equal to zero in this space of time periodic and time reversible solutions.

It is useful now to note that this condition is also equivalent to the invertibility of ∂T with the supremum norm. For that purpose, it is convenient to use Green functions for representing the inverse of ∂T. We have

$$\epsilon_\alpha(t) = \sum_\beta \int_0^{t_b} G_{\alpha,\beta}(t,\tau)\eta_\beta(\tau)d\tau \tag{31}$$

where $G_{\alpha,\beta}(t,\tau)$ is the time periodic and time reversible solution of eq. 30 for the sum of Dirac functions $\eta_\beta(t) = \sum_n (\delta(t+nt_b-\tau)+\delta(t+nt_b+\tau))$ and $\eta_\gamma(t) = 0$ for $\gamma \neq \beta$. The existence of these functions which are time periodic and time reversible with respect to t and τ, can be established with a proof similar to those described in ref. [13] for a single component case. In addition, these functions are continuous with respect to both variables. Their derivative with respect to t is defined except for $t = \tau$ and bounded. It is then straightforward to show that there exists a finite constant K such that

$$\sup_{\alpha,t}(|\epsilon_\alpha(t)|, |\dot{\epsilon}_\alpha(t)|, |\ddot{\epsilon}_\alpha(t)|) < K \sup_{\alpha,t}(|\eta_\alpha(t)| \tag{32}$$

which proves that $(\partial T)^{-1}$ is also bounded for the supremum norm on the functions and their first and second derivatives.

In the case where the number of components d of the oscillator is one, we can show that this property is equivalent to $d\omega(I)/dI \neq 0$. (This result should be published elsewhere in the context of linear stability problems of breathers.) When d is not equal to one, it is easy to check that the implicit function theorem (which will be applied in the next in a more complex case with infinitely many components), holds for a finite number of components. It shows that for any C^2 perturbation of the single oscillator Hamiltonian, the time periodic and time reversible trajectories which fulfill ∂T invertible can be continued up to a finite amplitude of this perturbation which proves structural stability.

The structural stability of a periodic orbit does not imply that it is linearly stable for small perturbations on the initial conditions. Actually, a structurally stable periodic orbit could be linearly stable or unstable.

4.2. Band Analysis

It is convenient to consider the complete spectral problem of eq. 30 which contains both the information concerning the linear stability of the orbits and the invertibility of ∂T. Since the time dependent coefficients

$V_{\alpha,\beta}(t) = \partial^2 V/\partial y_\alpha \partial y_\beta.(\mathbf{y}(t))$ are time periodic, the eigensolutions to this eigen equation have the Bloch-Floquet form $\epsilon_\alpha(t) = e^{i\theta t}\chi_\alpha(t)$ where $\chi_\alpha(t)$ is time periodic with period t_b. The eigenvalues of ∂T form a discrete set of continous branches $E_\sigma(\theta)$ which are 2π periodic and symmetric functions of θ. The intersections of these branches with the axis $\theta = 0$ yield the eigenvalues of the Sturm-Liouville operator with time periodic eigensolutions.

The time reversibility of the coefficients $V_{\alpha,\beta}(t)$ implies that at $\theta = 0$, the eigensolutions are either time symmetric or time antisymmetric. The condition for the structural stability of a periodic orbit, is that the eigenvalues at $\theta = 0$ corresponding to the time symmetric eigensolutions do not vanish.

Note that the time differentiation of eq. 27, yields always an eigensolution $\epsilon_\alpha = \dot{y}_\alpha$ of eq. 30 at $\theta = 0$ but it is time antisymmetric. The corresponding branch of eigenvalues $E_0(\theta)$ is tangent to the axis $E = 0$ for $\theta = 0$.

The linear stability of this periodic orbit is determined by eq. 30 for $E = 0$. The Floquet matrix $\mathcal{F}$ is the symplectic linear operator which is defined by integrating eq. 30 with $E = 0$ over a period of time t_b. It relates the trajectory coordinates $\{\epsilon_\alpha(t_b), \dot{\epsilon}_\alpha(t_b)\} = \mathcal{F}.\{\epsilon_\alpha(0), \dot{\epsilon}_\alpha(0)\}$ at time t_b to the initial conditions at time 0. The linear stability of the periodic orbit $\mathbf{y}(t)$ requires that no perturbation can grow exponentially in time. This condition is equivalent to say that all the eigenvalues of the Floquet matrix $\mathcal{F}$ are on the unit circle $e^{\pm i\theta_\sigma}$. The arguments θ_σ of these Floquet eigenvalues are just given by the intersections of the branches of eigenvalues $E_\sigma(\theta_\sigma) = 0$. The linear stability of the periodic orbits requires that there are precisely d pairs of intersections of the branches of eigenvalues of ∂T with $E = 0$ (see [6]). Contact points of tangent branches should be counted with their degeneracy which is generally two.

Therefore, it is quite helpful for understanding in practice what is going to happen after perturbation, to draw the graph of the branches of eigenvalues $E_\sigma(\theta)$ in the vicinity of the axis $E = 0$. We choose as an example a three dimensional potential:

$$V(\mathbf{y}) = \sum_{\alpha=1}^{3} \left(\frac{y_\alpha^2}{2} + \frac{y_\alpha^4}{4} \right) + \frac{C}{2}\left((y_2 - y_1)^2 + (y_3 - y_2)^2 + (y_1 - y_3)^2\right) \tag{33}$$

This 3d potential can be viewed as a finite ring of three coupled 1d anharmonic oscillators with periodic boundary conditions. For $\omega_b > 1$ and C not too large, this system has breather solutions which are obtained by continuation of solutions at $C = 0$. These breather solutions are time periodic and time reversible solutions of the three dimensional oscillator.

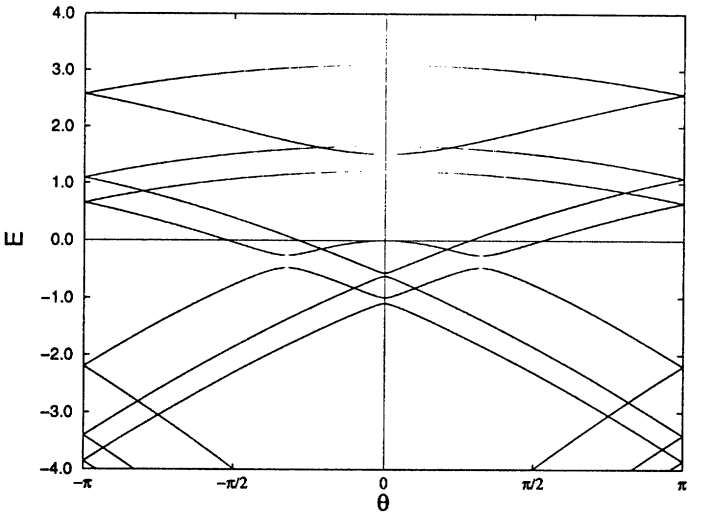

Fig. 1. – Branches of eigenvalues given by eq. 30 for the 3 dimensional oscillator with potential (33) for $C = 0.2$ and for a structurally stable periodic solution at $\omega_b = 1.5$ obtained by continuation versus C of the periodic solution at $C = 0$ where $y_1(t) \neq 0$ and $y_2(t) = y_3(t) \equiv 0$ (calculated by G. Kopidakis).

In that case, we can see 1- that the periodic orbit is structurally stable because there is only a unique branch tangent to $E = 0$ at $\theta = 0$ 2- that this periodic orbit is linearly stable because there are 3 pairs of intersections including the degenerate pair at $\theta = 0$.

5. MODEL EXAMPLES

In order to have a better representation of the classes of models we consider, let us now give two simple examples of models with and without piezo active couplings which has straightforward d dimensional extensions.

5.1. Model 1 with piezoactive coupling

This model consists of a chain of atoms with a diatomic molecule in each unit cell with two atoms with mass m_1 and m_2 which are coupled anharmonically by potential $V(x)$. It is represented schematically in a 2d case on figure 2. Only the nearest neighbor atoms of neighboring molecules are coupled harmonically with the constant C.

$$\mathcal{H}_1 = \sum_i \frac{m_1}{2}\dot{u}_i^2 + \frac{m_2}{2}\dot{v}_i^2 + V(v_i - u_i) + \frac{C}{2}(u_i - v_{i-1})^2 \qquad (34)$$

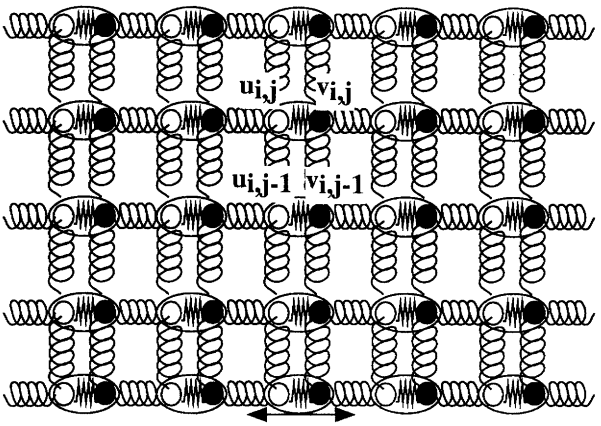

Fig. 2. – Schemes of Model 1 in two dimensions.

We can put this Hamiltonian in the general form (1) by defining the distortion of each molecule $y_i = v_i - u_i$ and its center of mass $x_i = (m_1 u_i + m_2 v_i)/(m_1 + m_2)$. The 1d Hamiltonian is then

$$\begin{aligned}\mathcal{H}_1 = \sum_i & \frac{1}{2}(m_1+m_2)\dot{x}_i^2 + \frac{C}{2}(x_i - x_{i-1})^2 \\ & + \frac{1}{2}\frac{m_1 m_2}{m_1+m_2}\dot{y}_i^2 + V(y_i) + \frac{C}{2}y_i^2 - \frac{C}{2}\frac{m_1 m_2}{(m_1+m_2)^2}(y_i - y_{i-1})^2 \\ & + \frac{C}{m_1+m_2}y_i(-m_1 x_{i+1} + (m_1 - m_2)x_i + m_2 x_{i-1}) \end{aligned} \tag{35}$$

The Fourier transform of the coupling matrix $\mathbf{P}$ which has only one component here is

$$P(q) = \frac{C}{m_1+m_2}((m_1 - m_2)(1 - \cos q) - i(m_1+m_2)\sin q) \tag{36}$$

which is equivalent to $-iCq$ for $q \to 0$. As a result, the internal mode of the molecule is piezoactive. The same result holds for the same model in higher dimensions.

5.2. Model 2 without piezoactive coupling

This model now consists of two chains of atoms with a diatomic molecule in each unit cell with again two atoms with mass m_1 and m_2 which are

coupled anharmonically by potential $V(x)$. It was used for simple modeling of DNA chains in ref. [12].

$$\mathcal{H}_2 = \sum_i \frac{m_1}{2}\dot{u}_i^2 + \frac{m_2}{2}\dot{v}_i^2 + V(v_i - u_i) + \frac{C_1}{2}(u_i - u_{i-1})^2 + \frac{C_2}{2}(v_i - v_{i-1})^2 \tag{37}$$

As before the distortion of each molecule is $y_i = v_i - u_i$ and its center of mass is $x_i = (m_1 u_i + m_2 v_i)/(m_1 + m_2)$. In [12], u_i and v_i represent the displacement of DNA bases transverse to the trends, and $V(v_i - u_i)$ is the anharmonic potential resulting from the hydrogen bonds between the trends. The Hamiltonian is then

$$\mathcal{H} = \sum_i \frac{1}{2}(m_1 + m_2)\dot{x}_i^2 + \frac{C_1 + C_2}{2}(x_i - x_{i-1})^2 + \frac{1}{2}\frac{m_1 m_2}{m_1 + m_2}\dot{y}_i^2 + V(y_i) + \frac{1}{2}\frac{C_1 m_2^2 + C_2 m_1^2}{(m_1 + m_2)^2}(y_i - y_{i-1})^2 + \frac{C_2 m_1 - C_1 m_2}{m_1 + m_2}(x_i - x_{i-1})(y_i - y_{i-1}) \tag{38}$$

This model has the form 1. We get

$$P(q) = 2\frac{C_2 m_1 - C_1 m_2}{m_1 + m_2}(1 - \cos q) \tag{39}$$

which is equivalent to $(C_2 m_1 - C_1 m_2)/(m_1 + m_2).q^2$ for $q \to 0$. In this model, the internal mode of the molecule is not piezoactive.

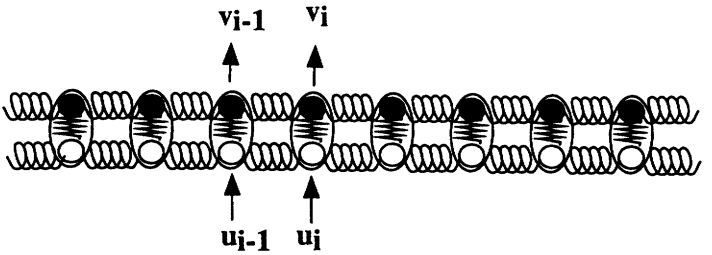

Fig. 3. – Scheme of Model 2 in one dimension.

6. PROOF FOR THE EXISTENCE OF PIEZOACTIVE BREATHERS

As in the initial paper [3], our existence proof is based on the continuation of the breather solutions which trivially exist at the anticontinuous limit. In the present case, our method involves first the elimination of the harmonic variables $\mathbf{X}(t)$ in eqs. 6 from eq. 5.

For the piezoactive anharmonic modes defined in subsection (3.1), we cannot use the supremum norms as we did previously because this emimination involves operator $\mathbf{S}_0$ which is not bounded for that norm. However, since it is bounded for the l_2 norm, it appears that it remains possible to use the implicit function theorem in the Banach space defined with the L^2 norm. As a result, we shall obtain the proof of continuation for breathers and multibreathers involving a finite number of piezoactive breathers only.

The l_2 norm of multibreathers with infinitely many piezoactive breathers is not defined and because we cannot switch to the supremum norm, we cannot use our method to prove that they can be continued from their anticontinuous limit. Actually, we believe that this continuation is impossible (in general) for physical reasons. The reason is that the absence of bound for the supremum norm of operator $\mathbf{S}_0$ is related to the possible existence of configurations with infinitely many breathers which generate divergent stresses at finite distance in the crystal.

In contrast, we shall see in the next section that for nonpiezoactive breathers, we can use either the l_2 norm or the supremum norm.

6.1. Definition of operating subspaces

It is convenient to define first, the two spaces of functions which we shall use use for applying the implicit function theorem to the continuation of the piezoactive breathers.

The space denoted $\mathcal{E}_S^0(\omega_b)$ is defined by arrays of functions $\mathbf{F}(t) = \{f_{i,\alpha}(t)\}$ which are time periodic with the given period $t_b = 2\pi/\omega_b$ and time reversible:

$$f_{i,\alpha}(t + t_b) = f_{i,\alpha}(t) \quad \text{and} \quad f_{i,\alpha}(t) = f_{i,\alpha}(-t) \tag{40}$$

We also require that $\mathbf{F}(t)$ is square summable in order that $\mathcal{E}_S^0(\omega_b)$ is a Banach space for the L^2 norm

$$(\|\mathbf{F}(t)\|_2)^2 = \frac{\omega_b}{2\pi} \sum_{\mathbf{n},\alpha} \int_0^{t_b} |f_{\mathbf{n},\alpha}(t)|^2 dt \tag{41}$$

We also consider the subspace $\mathcal{E}^2_S(\omega_b)$ of arrays of functions $\mathbf{Y}(t) = \{y_{i,\alpha}(t)\}$ which are also twice differentiable. It is also a Banach space with the norm

$$(\|\mathbf{Y}(t)\|_{2,2})^2 = (\|\mathbf{Y}(t)\|_2)^2 + (\|\dot{\mathbf{Y}}(t)\|_2)^2 + (\|\ddot{\mathbf{Y}}(t)\|_2)^2 \qquad (42)$$

6.2. Elimination of the Harmonic variables

Let us consider ω_b such that no harmonic $p\omega_b$ belongs to the phonon spectrum of system defined by eq. 11 for any $p \neq 0$.

We consider solutions of eqs. (5) and (6) such that $\mathbf{Y}(t) \in \mathcal{E}^2_S(\omega_b)$. This condition means that we shall consider only spatially localized solutions for the variable $\mathbf{Y}(t)$ but not for $\mathbf{X}(t)$.

No conditions are required for $\mathbf{X}(t)$ since equation (5) determines the harmonic variables $\mathbf{X}(t)$ as a linear function of $\mathbf{Y}(t)$. Up to an arbitrary uniform translation of the crystal, this determination is unique. The time Fourier components defined as

$$\mathbf{X}^p = \frac{\omega_b}{2\pi}\int_0^{t_b} \mathbf{X}(\tau)e^{-ip\omega_b\tau}d\tau \qquad \text{and} \qquad \mathbf{Y}^p = \frac{\omega_b}{2\pi}\int_0^{t_b} \mathbf{Y}(\tau)e^{-ip\omega_b\tau}d\tau \qquad (43)$$

are related by the equation

$$\mathbf{X}^p = -k\mathbf{R}_p.\mathbf{Y}^p \qquad (44)$$

where operator $\mathbf{R}_p$ is defined as

$$\mathbf{R}_p = \left(\mathbf{N} - p^2\omega_b^2\mathbf{M}\right)^{-1}.\mathbf{P}^t \qquad (45)$$

The time reversibility implies that the Fourier coefficients of $\mathbf{Y}(t)$ are real and since the matrices $\mathbf{R}_p$ are real, the Fourier coefficients of $\mathbf{X}(t)$ also real, that is $\mathbf{X}(t)$ is time reversible.

For $p \neq 0$, operators $\mathbf{R}_p$ are well defined with a finite norm in l^2 since ω_b and its harmonic $p\omega_b$ have been assumed to be not in the phonon spectrum. In contrast, for $p = 0$ and when the breather mode is piezoactive, operator $\mathbf{R}_0$ considered in eq. 15 is unbounded for the l^2 norm and thus is not well defined. Actually, since the quantity which appears in eq. 6 is $\mathbf{Z}(t) = \mathbf{P}.\mathbf{X}(t)$ we do not need to use this operator but the linear operator $\mathcal{S}$:

$$\mathbf{Y}(t) \to \mathbf{Z}(t) = \mathbf{P}.\mathbf{X}(t) = \mathcal{S}.\mathbf{Y}(t) \qquad (46)$$

Defining the time Fourier coefficients as $\mathbf{Z}(t) = \sum_p \mathbf{Z}^p e^{ip\omega_b t}$ with p integer, we readily get $\mathbf{Z}^p = \mathbf{S}_p.\mathbf{Y}^p$ with

$$\mathbf{S}_p = -\frac{1}{p^2}\mathbf{P}.\left(\omega_b^2\mathbf{M} - \frac{1}{p^2}\mathbf{N}\right)^{-1}.\mathbf{P}^t \tag{47}$$

Eq. 6 can be written as

$$m\ddot{y}_{\mathbf{n},\alpha} + \frac{\partial V(\mathbf{y_n})}{\partial y_{\mathbf{n},\alpha}} - k^2(\mathcal{S}.\mathbf{Y}(t))_{\mathbf{n},\alpha} + k'\frac{\partial \mathbf{W}(\mathbf{Y}(t))}{\partial y_{\mathbf{n},\alpha}} = 0 \tag{48}$$

We have shown above that for a realistic crystal model, $\mathbf{S}_0$ defined by eq. 15 is always bounded for the l^2 norm and since ω_b and its harmonic are not in the phonon spectrum of the crystal, $\mathbf{S}_p$ are also bounded for the norm l^2. In addition, the l^2 norm of $\mathbf{S}_p$ goes to zero for $p \to \infty$ as $\|\mathbf{P}.\mathbf{M}^{-1}.\mathbf{P}^t\|_2/(p\omega_b)^2$. We now show that operator $\mathcal{S}$ is also bounded for the norm L^2.

The square of the L^2 norm $\|\mathbf{Y}(t)\|_2$ of $\mathbf{Y}(t)$ defined by (41) can be readily written as the sum of the squares of the l^2 norms of its Fourier coefficients

$$(\|\mathbf{Y}(t)\|_2)^2 = \sum_p (\|\mathbf{Y}^p\|_2)^2 \tag{49}$$

$(\|\mathbf{Y}^p\|_2)^2 = \sum_{\mathbf{n},\alpha} |y^p_{\mathbf{n},\alpha}|^2$ is the square of the l^2 norm of $\mathbf{Y}^p$.

Then, we can write

$$\begin{aligned}
&(\|\mathcal{S}.\mathbf{Y}(t)\|_2)^2 = \sum_p (\|\mathbf{S}_p.\mathbf{Y}^p\|_2)^2 \\
&\leq \sum_p (\|\mathbf{S}_p\|_2)^2(\|\mathbf{Y}^p\|_2)^2 \leq (\sum_p (\|\mathbf{Y}^p\|_2)^2)(\sum_p (\|\mathbf{S}_p\|_2)^2) \\
&= (\|\mathbf{Y}(t)\|_2)^2\left((\|\mathbf{S}_0\|_2)^2 + \sum_{p\neq 0}\frac{1}{p^4}\left(\|\mathbf{P}.\left(\omega_b^2\mathbf{M} - \frac{1}{p^2}\mathbf{N}\right)^{-1}.\mathbf{P}^t\|_2\right)^2\right)
\end{aligned} \tag{50}$$

The sum in the last member of ineq. 50 is convergent, which proves that

$$\|\mathcal{S}\|_2 = \sup_{\mathbf{Y}\in\mathcal{E}_S^0} \frac{\|\mathcal{S}.\mathbf{Y}(t)\|_2}{\|\mathbf{Y}(t)\|_2} < \infty \tag{51}$$

Since $\|\mathbf{Y}(t)\|_2 \leq \|\mathbf{Y}(t)\|_{2,2}$ defined by eq. 42, $\mathcal{S}$ is also bounded when $\mathcal{E}_S^2(\omega_b)$ and $\mathcal{E}_S^0(\omega_b)$ are considered with the norms defined in subsection (6.1).

6.3. Definition of a map

The first member of eq. 48 defines a nonlinear map $\mathbf{F}(t) = \mathcal{T}(k,k')(\mathbf{Y}(t))$ where $\mathbf{F}(t) = \{f_{\mathbf{n},\alpha}(t)\}$ is given by

$$f_{\mathbf{n},\alpha}(t) = m\ddot{y}_{\mathbf{n},\alpha} + \frac{\partial V(\mathbf{y_n})}{\partial y_{\mathbf{n},\alpha}} - k^2(\mathcal{S}.\mathbf{Y}(t))_{\mathbf{n},\alpha} + k'\frac{\partial \mathbf{W}(\mathbf{Y}(t))}{\partial y_{\mathbf{n},\alpha}} \qquad (52)$$

It depends on the two parameters k and k'. We prove that it is a continuous map from the Banach space $\mathcal{E}^2_S(\omega_b)$ (with the norm (42) into the wider Banach space $\mathcal{E}^0_S(\omega_b)$ with the norm (41)).

For that purpose, we prove first that $\mathbf{Y}(t) \in \mathcal{E}^2_S(\omega_b)$ implies that $\mathbf{Y}(t)$ and $\dot{\mathbf{Y}}(t)$ are also bounded for the supremun norm. Indeed, considering for example $\|\mathbf{Y}(t)\|_s = \sup_{\mathbf{n},\alpha} |y_{\mathbf{n},\alpha}(t)|$, we can write using the Schwarz inequality

$$\begin{aligned}
|y_{\mathbf{n},\alpha}(t)| &= |\sum_p y^p_{\mathbf{n},\alpha} e^{ip\omega_b t}| \leq |y^0_{\mathbf{n},\alpha}| + \sum_{p\neq 0} \frac{1}{|p|}.|py^p_{\mathbf{n},\alpha}| \\
&\leq \|\mathbf{Y}(t)\|_2 + \left(\sum_{p\neq 0}\frac{1}{p^2}\right)^{1/2}.\left(\sum_{p\neq 0}|py^p_{\mathbf{n},\alpha}|^2\right)^{1/2} \\
&\leq \|\mathbf{Y}(t)\|_2 + \frac{\pi}{\sqrt{3}}\|\dot{\mathbf{Y}}(t)\|_2 \\
&\leq \frac{\pi}{\sqrt{3}}\|\mathbf{Y}(t)\|_{2,2} = B(\mathbf{Y}) \qquad (53)
\end{aligned}$$

where the last bound $B(\mathbf{Y})$ is independent of $\mathbf{n}$ and α. The condition $|y_\alpha| \leq B(\mathbf{Y})$ for all α defines the ball $\mathcal{B}(\mathbf{Y})$ for $\mathbf{y}$.

Then using the fact that function $V(\mathbf{y})$ is C^2, it comes out that

$$z_{\mathbf{n},\alpha}(t) = \frac{\partial V(\mathbf{y_n})}{\partial y_{\mathbf{n},\alpha}} \qquad (54)$$

is also L^2 since we can write $|z_{\mathbf{n},\alpha}(t)| < K_1|y_{\mathbf{n},\alpha}(t)|$ where

$$K_1 = \sup_{\alpha,\mathbf{y}\in\mathcal{B}(\mathbf{Y})}\left(\sum_\beta \left|\frac{\partial^2 V(\mathbf{y})}{\partial y_\alpha \partial y_\beta}\right|^2\right)^{\frac{1}{2}} \qquad (55)$$

Since the functions $W_{\mathbf{k}-\mathbf{l}}(\mathbf{y_k},\mathbf{y_l})$ in eq. 4 which describe the direct nearest neighbor interaction between the molecules, are also assumed to be C^2,

it is found similarly that $\frac{\partial \mathbf{W}(\mathbf{Y}(t))}{\partial y_{\mathbf{n},\alpha}}$ in eq. 52 is L^2. As a result, $f_{\mathbf{n},\alpha}(t)$ in eq. 52 is also L^2.

Using the bounds on $\mathbf{Y}(t)$ and the C^2 property of the potentials of the model, it becomes straightforward to prove that $\mathcal{T}(k,k')$ is a continuous map between the Banach spaces $\mathcal{E}_S^2(\omega_b)$ and $\mathcal{E}_S^0(\omega_b)$ for their respective norms. It is also differentiable and its derivative linear operator denoted $\{\eta_{\mathbf{n},\alpha}\} = \partial\mathcal{T}(k,k',\mathbf{Y}).\{\epsilon_{\mathbf{n},\alpha}\}$ depends continuously on $\mathbf{Y}(t)$ and k,k'.

6.4. The implicit function theorem

Now, we have established all the properties which allow the application of the implicit function theorem. We recall its general statement [13]:

Let E,F,G be three Banach spaces, f maps an open set A in $E \times F$ into G and is continuously differentiable. Let x_0, y_0 such that $f(x_0,y_0)=0$ and such that $D_2 f(x_0,y_0)$ be a linear homeomorphism of F into G. Then, there exists a neighborhood U_0 of x_0 in E such that for any open set U in U_0 containing x_0, there exists a unique map $u(x)$ of U into F such that $u(x_0)=y_0$ and $(x,u(x))$ is in A and $f(x,u(x))=0$. In addition, $u(x)$ is continuously differentiable.

With ω_b fulfilling the nonresonance conditions described in subsection (4.1), we choose $E=\mathcal{R}^2$, the space of parameters (k,k'), $F=\mathcal{E}_S^2(\omega_b)$, $G=\mathcal{E}_S^0(\omega_b)$ and the map $f=\mathcal{T}(k,k')(\mathbf{Y}(t))$. The open set $A=E\times F$ is the whole product space.

For $k=k'=0$, this map has trivial zeros in $\mathcal{E}_S^2$, which are obtained by choosing an arbitrary but *finite* number of oscillators (finite multibreathers) which are oscillating with a given structurally stable time reversible and time periodic solution $\mathbf{y}(t)$ with period t_b which fulfills the nonresonance conditions (4.1). The phase of the oscillators which are moving can be arbitrarily zero or π that is we choose $\mathbf{y}(t)$ or $\mathbf{y}(t+t_b/2)$.

For each of these zeros of $\mathcal{T}(k,k')$ at $k=k'=0$, the linear derivative operator $\partial\mathcal{T}(k,k')$ is invertible with the appropriate L^2 norms because it becomes a direct product of three kinds of operators which are defined by eq. 30 either for the rest solution $\mathbf{y}(t)=\mathbf{0}$ or for the time reversible and time periodic solution $\mathbf{y}(t)$ (phase 0) or $\mathbf{y}(t+t_b/2)$ (phase π). One of these operators maps $\mathbf{y}_\mathbf{n}(t)$ in the $\mathbf{n}$ component subspace of $\mathcal{E}_S^2$ into $\mathbf{f}_\mathbf{n}(t)$ in the corresponding subspace of $\mathcal{E}_S^0$. Each of these operators is invertible as a direct consequence of the nonresonance conditions (4.1) and the structural stability assumption. The norm of the global inverse which operates from the direct sum $\mathcal{E}_S^0$ into $\mathcal{E}_S^2$ is bounded by the supremum of the norm of the three inverse operators and thus is finite.

Then, all the conditions required for the theorem, are fulfilled. The continuation of this multibreather solution holds for (k, k') in a neighborhood of $(0, 0)$, that is for k and k' not too large.

6.5. Noncontinuation of some infinite multibreather configurations

The extension of the open domain in (k, k') where the continuation holds, depends on the initial finite multibreather. When the number of piezoactive breathers in the considered multibreather state at the anticontinuous limit, is infinite, our continuation theorem does not hold in principle because the solution we consider, is not in $\mathcal{E}_S^2$.

There is a physical reason for this mathematical condition. Indeed, the static component of the atomic displacements $\mathbf{x}_\mathbf{n}^0$ which would be generated by the breathers, could become infinite because of eq. 20 and thus undefined. Actually, this divergency does not necessarily make physically any problem because one could well accept macroscopic deformation of the crystal. However, a problem occurs in two dimensions and more, because the stress $\mathbf{S}_0.\mathbf{Y}^0$ which would be generated by the static component of the breathers might not be bounded because we have shown in subsection (3.1), that operator $\mathbf{S}_0$ is not bounded for the supremum norm. It is known that similarly, clusters of impurities which do not preserve the volume of a harmonic crystal, generate divergent stresses, when their size grows. As an example, we show a configuration of piezoactive breathers on figure 4 where such a situation occurs.

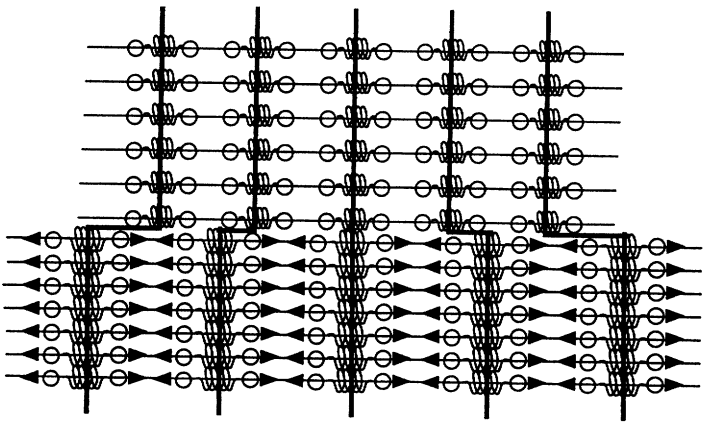

Fig. 4. – A distribution of piezoactive breathers in a 2d crystal of diatomic molecules which cannot be continued from the anticontinuous limit. The size of the unit cell is changed in the region occupied by the breathers (lower part). For an infinite system, the mismatch between the two parts of the crystal generate unbounded *relative* atomic displacements and unbounded stresses.

Actually, real crystals are not harmonic and this divergent stress does not occur because it is relaxed by the formation of dislocations and cracks in the crystal. However, our model cannot generate any defect because we assumed that the acoustic phonons are harmonic. For that reason, the general proof of continuation of infinite clusters of breathers is not possible from the anticontinuous limit of our model. However, we conjecture that there are distributions of infinitely many breathers which could be continued from the anticontinuous limit, but these distributions should be chosen sufficiently "homogeneous" in order that the stress they generate in the crystal be uniformly bounded.

7. PROOF OF THE EXISTENCE OF NONPIEZOACTIVE MULTIBREATHERS

The above continuation proof holds *a fortiori* for multibreathers involving non piezo active breathers defined in subsection (3.2). However, the existence proof can be extended as well for multibreathers involving an infinite number of nonpiezoactive breathers by using the fact that operator $\mathbf{S}_0$ is bounded for the supremum norm (see subsection (3.2)). This proof also holds for the piezoactive breathers in one dimensional models because in that case, operator $\mathbf{S}_0$ remains bounded for the supremum norm.

We redefine the new Banach spaces $\mathcal{E}_S^{0,s}(\omega_b)$ as the vectorial space of C^0 functions $\mathbf{F}(t) = \{f_{i,\alpha}(t)\}$ which are time periodic with the given period $t_b = 2\pi/\omega_b$ and time reversible: with the standard supremum norm

$$\|\mathbf{F}\|_s = \sup_{i,p,\alpha,t} (|F_{i,p,\alpha}(t)|) \tag{56}$$

The new Banach space $\mathcal{E}_S^{2,s}(\omega_b)$ is defined identically but the functions $\mathbf{Y}(t) = \{y_{i,\alpha}(t)\}$ are assumed to be C^2 and

$$\|\mathbf{Y}\|_{s,2} = \sup \left(\|\|\mathbf{Y}\|_s, \|\|\dot{\mathbf{Y}}\|_s, \|\|\ddot{\mathbf{Y}}\|_s \right) \tag{57}$$

Operator $\mathcal{S}$ can be formally defined as in subsection (6.2) but we have now to prove that it is bounded for the supremum norm. It is convenient to rewrite $\mathcal{S}$ as a series

$$\mathcal{S} = \sum_p e^{ip\omega_b t} \mathbf{S}_p \mathcal{P}_p \tag{58}$$

where $\mathcal{P}_p.\mathbf{Y}(t) = \mathbf{Y}^p$ is the projector which yields the p Fourier component (43) of $\mathbf{Y}(t)$. Each operator $\mathbf{S}_p$ in the series (58) is bounded for the supremum norm: $\mathbf{S}_0$ is bounded because we consider nonpiezoactive modes as explained in subsection (3.2). For $p \neq 0$, the Fourier transform $\mathbf{S}^p(\mathbf{q})$ of $\mathbf{S}_p$ defined by eq. 47 is

$$\mathbf{S}^p(\mathbf{q}) = -\mathbf{P}(\mathbf{q}).\left(p^2\omega_b^2\mathbf{M} - \mathbf{N}(\mathbf{q})\right)^{-1}.\mathbf{P}^t(\mathbf{q}) \tag{59}$$

The finite inverse matrix in eq. 59 is well defined since for any $p \neq 0$, $p\omega_b$ does not belong to the phonon spectrum defined by eq. 11. Consequently, $\mathbf{S}^p(\mathbf{q})$ is a C^2 function of $\mathbf{q}$ which implies that the Fourier series which defines $\mathbf{S}^p(\mathbf{q})$ is absolutely convergent (C^0 would be enough). As a result, $\mathbf{S}^p$ is bounded for the supremum norm. In addition, for $p \to \infty$, $\|\mathbf{S}^p\|_s \simeq \|\mathbf{P}.\mathbf{M}^{-1}.\mathbf{P}^t\|_s/(p^2\omega_b^2)$ which implies that the series involved in the inequality

$$\|\mathcal{S}\|_s \leq \|\mathbf{S}_0\|_s + \sum_{p\neq 0} \|\mathbf{S}_p\|_s < \infty \tag{60}$$

is convergent and $\mathcal{S}$ is bounded for the supremum norm. This is *a fortiori* true when $\mathcal{S}$ is considered as a map from $\mathcal{E}_S^{2,s}(\omega_b)$ to $\mathcal{E}_S^{0,s}(\omega_b)$.

We also need to check that each of the local operators defined by eq. 30 is also invertible for the supremum norm. Actually, we proved in subsection 4.1 that the invertibility of these local operators for the L^2 norm is equivalent to their invertibility for the supremum norm.

It is now straightforward to check that the operator $\mathcal{T}(k, k')$ defined by eq. 52, but from the space $\mathcal{E}_S^{2,s}(\omega_b)$ into the space $\mathcal{E}_S^{0,s}(\omega_b)$ with their respective norms, is continuous, and is differentiable with a continuous derivative operator. The conditions for the application of the implicit function theorem hold for any infinite or finite multibreather state which is in $\mathcal{E}_S^{2,s}(\omega_b)$ for $k = k' = 0$.

8. EXTENSIONS AND DISCUSSIONS

Our approach can be easily extended to even more complex models (but however still suffers some limitations). It suffices that the variables which describe the crystal configuration can be split in two categories:

• The optical variables which are unchanged by crystal translations, and are anharmonic.

• The acoustic variables which are uniformly shifted when the crystal is translated.

The part of the Hamiltonian involving the acoustic variables has to be harmonic.

It comes out that the number of optical variables in the unit cell involved in the displacement vector $\mathbf{y_n}(t)$ and which are considered as anharmonic is not necessarily d but any number which is of course finite. However, we should have at least d variables describing the acoustic variables in a realistic d dimensional crystal. According to previous study on optical breathers [Aub97], the condition of time reversibility can be relaxed.

8.1. Non time reversible solutions, rotating molecules-rotobreathers

The assumption of time reversibility for the breathers and multibreathers we considered, implies that the molecular motions are only oscillations. However, we may also consider nontime reversible solutions. For example, at the anticontinuous limit, single molecules may have time periodic solutions in their local potential which correspond to rotations.

We can prove the possible continuation of nontime reversible solutions with the same methods which were used in ref. [6] for purely optical breathers. We sketch here the methods we used.

In the first method, we search for solutions of eqs. 5 and 6 in the space $\mathcal{E}_A^2$ or $\mathcal{E}_A^{2,s}$ which are defined identically to $\mathcal{E}_S^2$ or $\mathcal{E}_S^{2,s}$ in subsection (6.1) but where the time reversibility condition is replaced by a time antisymmetry condition. The proofs made above works identically just by exchanging the condition of time reversibility with the condition of time antisymmetry. This method is only applicable when the Hamiltonian itself is time reversible.

The second method is based on the concept of effective action. It could be used for Hamiltonians which are not time reversible, for example when a magnetic field is involved and the crystal contains charged ions. However, in our extended model, we cannot use the action angle representation as in ref. [6]. Nevertheless, for the periodic orbit $\mathbf{y}(t)$ with period t_b of a molecule at the continuous limit which is rotating around some axis, we can define the angle $\theta(t)$ of the molecule projected in the plane perpendicular to this axis. This angle $\theta(t)$ fulfills (for example) the condition $\theta(t+t_b) = \theta(t) + 2\pi$. Then, we define the average angle $\alpha = \int_0^{t_b} (\theta(t) - \omega_b t)dt/t_b$ during one revolution.

Then, we proceed as in [6] by extremalizing the action of the system in the space of time periodic orbits but with fixed average angles for the rotating molecules. We extremalize this action in the space $\mathcal{E}^2(\{\alpha_{\mathbf{n}}\})$ or $\mathcal{E}^{2,s}\{\alpha_{\mathbf{n}'}\})$ defined as in subsection (6.1) but where the molecules at the sites denoted $\mathbf{n}'$ which have been selected to rotate at the anticontinuous limit, have fixed average angle $\{\alpha_{\mathbf{n}'}\}$.

Since the harmonic variables $\mathbf{x}_{\mathbf{n}}(t)$ can be eliminated identically by the operator $\mathcal{S}$ (which actually does not require time reversibility conditions to be defined), the continuation theorems proved above still hold for piezoactive as well as for nonpiezoactive rotobreathers, in their respective subspaces (under the same conditions of nonresonance and structural stability). Moreover, the constraint parameters $\{\alpha_{\mathbf{n}'}\}$ can be incorporate in the Banach space of parameters E appearing in the implicit function theorem, which implies that this continuation is uniform with respect to the constraints [6].

Since we have constraints, these solutions are not true extrema of the action and thus are not true solutions of the dynamical system (but only ghost solutions). The resulting extremalized action is a function of the average angles of the molecules called the effective action. This function is obviously invariant by a global rotation of the average molecule angles which just corresponds to change the time origin. It is 2π periodic with respect to each phase $\alpha_{\mathbf{n}'}$. and then, it has at least 2^{P-1} extrema apart a time translation. Each of these extrema corresponds to real solutions of eqs. 5 and 6 which are called multirotobreathers. The single rotobreather is obtained when only one molecule rotating in the whole crystal.

By this method, we can also build multibreather or multirotobreather solutions with phase torsion as we did in [18]. However, since for piezoactive breathers (or rotobreathers), the number of breathers (or rotobreathers) is finite, we shall get only vortices or multivortices in energy flow.

8.2 Breathers in random networks with acoustic phonons

Instead of a crystal, we can assume that we have a random network in d dimensions where each site is connected to neighboring sites the number of which is finite and bounded. At each site we attach molecules which are not necessarily identical. The anharmonic molecule at site $\mathbf{n}$, is submitted to the local potential $V_{\mathbf{n}}(\mathbf{y}_{\mathbf{n}})$ where its internal coordinates are represented by the vector $\mathbf{y}_{\mathbf{n}}$ with a finite number of components. The local potential and the number of components may depend on $\mathbf{n}$.

There are also harmonic variables $\mathbf{x_m}$ which are attached to a different random network $\mathbf{m}$ different but superposed to the network of molecule. The Hamiltonian of this system is decomposed as in the periodic case eq. 1 as the sum of four terms.

H_{elst} is a harmonic hamiltonian for a random elastic network, the energy of which is invariant by global translations of the atomic coordinates in the d directions of the space. It is represented by a mass matrix $\mathbf{M}$ and an elasticity matrix $\mathbf{N}$ which acts on the global vector $\mathbf{X} = \{\mathbf{x_m}\}$. Both matrices may have arbitrary coefficients but we shall have to introduce global constraint to insure the stability of the network.

H_{AC} is the Hamiltonian of anharmonic uncoupled oscillators corresponding to the internal vibrations of the molecule with masses which can be also arbitrary.

Furthermore, there is a harmonic coupling between the set of variables $\mathbf{X}$ and the set $\mathbf{Y} = \{\mathbf{y_n}\}$ of internal coordinates described by the matrix $\mathbf{P}$ which also can have arbitrary coefficients. The amplitude of this coupling is tuned by the coefficient k. Finally, there is also a direct coupling between neighboring anharmonic oscillators.

It is a priori difficult to define the sound velocities in such a system because of the randomness of the network and the interactions do not allow one to use space Fourier transformations. However, for a realistic model, the sound velocities should remain well defined quantities as in glasses for example.

However, it is possible to shortcut complex considerations about the hypotheses which should be fulfilled by the model. We just make directly the assumption that the l^2 norm of the product $\mathbf{S}_0 = \mathbf{P}.\mathbf{N}^{-1}.\mathbf{P}^t$ is finite. This assumption means that as for a regular spring, the energy induced by any optical distortion of the molecule remains of the order of the sum of the square of the distortion. This assumption is physically necessary to have a realistic model because it just says that the stiffness of the system for any distortion of the optical modes is *finite*. In case the initial model would not have this property, this would mean that the model has not been properly defined for describing a physical system, and should be discarded (by physicist's).

Once this assumption is made, the proof for the existence of piezoactive breathers works identically to the crystal case, with of course the same assumptions. We have first the nonresonance conditions which assume that for $p \neq 0$, the breather harmonic $p\omega_b$ do not belong neither to the global acoustic phonon spectrum nor to the optical phonon spectrum (which now has been broadened because of the randomness of the molecular oscillators).

The second assumption is that at the anticontinuous limit, the multibreather solutions only involves structurally stable orbits for the local oscillators which have been selected to move at the anticontinuous limit.

8.3 More anharmonicity?

Our theory is limited by the necessary assumption that the acoustic phonons must be treated harmonically. Could we abandon this assumption? We think that this should be possible if the anharmonicity in the acoustic phonons (and their coupling with the optical modes) are chosen properly for having a physically acceptable crystal. Although the sound velocities could be defined by considering the harmonic parts of these interaction, it is not simple to express the stability condition of the crystal because the phonon gap is vanishing.

A possible formulation would be that the harmonic part of the Hamiltonian be perturbed by higher order terms which preserve its convexity in a certain neighborhood of the equilibrium steady state of the crystal (to be defined). Then, it could be possible to prove that the operator $\mathcal{S}$ we defined here in the harmonic case in eq. 46, could be continued as a L^2 operator up to an anharmonic perturbation not too large by using again the implicit function theorem. In summary, we conjecture that the existence of breathers in models with acoustic phonons should not be subjected to the harmonicity of these acoustic phonons and of their coupling. Breathers may exist in the most general models of anharmonic crystals.

The approach suggested by R. MacKay [11] considers models where all the interactions are anharmonic and thus should be more general than the proof we presented here. However, the detailed proof of the existence of breathers in these most general models with anharmonic acoustic phonons has not been yet published but may suffer some criticismes.

We briefly discuss the basic ideas of this approach from what we know and in view of our results. In principle, it is formally elegant and does not require the elimination of acoustic variables as we did here but consider the whole set of atomic coordinates. The anticontinuous limit is obtained as in [10] when the ratio of the masses of two kinds of atoms goes to zero. Two configurations which are related by spatial translation or rotation are considered as equivalent. Then, a norm is defined in this space of equivalence classes of configurations which only involves the relative distance of the atoms on some "triangulation" of the lattice. It is chosen in order that the distances between nearest neighbour atoms on this triangulation determine uniquely the atomic configuration. Then it is claimed [11] that the implicit function theorem should hold in the Banach

space of time periodic and time reversible configurations considered with this norm. As far as we know, it is also claimed that there are several norms which could be used equivalently for this approach which are for example a supremum norm, a l^2 norm or else. In case the breathers are piezoactive, this assertion contradicts our results because it would allows one to continue any infinite multibreather configuration which we know to be untrue [6]. At the present stage, this new approach did not recognized yet the role of the piezoactivity for breathers in their continuation but it can be considered as promising if more appropriate norms could be chosen which we nevertherless believe to be possible.

9. BREATHER STABILITY AND HARMONIC DECAYS

We should complete this paper by a discussion of two important properties concerning these breather solutions. One concerns the decays of the breather harmonic at long distance and the second their linear stability. For brevity, we only sketch here physicist arguments which should be easy to to turn into rigorous proofs.

9.1 Exponential decay of the dynamical part of the breathers

As we have seen above, breathers and multibreathers in systems with acoustic phonons generally generate long range distortions which do not decay as exponentials. Actually, this problem concerns essentially the static component. For single breathers or multibreathers involving a finite number of breathers, the dynamical Fourier components $\mathbf{x}_{\mathbf{n}}^{p}(t)$ and $\mathbf{y}_{\mathbf{n}}^{p}(t)$ for $p \neq 0$, are expected to decay exponentially in realistic models.

However, the conditions we assumed in subsection (2.2), that the acoustic interactions are not too much long range is too loose. The assumption that the matrices $\mathbf{N}(\mathbf{q})$ and $\mathbf{P}(\mathbf{q})$ are C^2 functions of the wavevector $\mathbf{q}$ is not sufficient, because it allows long range interactions between the atoms which decay as power laws and thus compromises a fast exponential decay of the breather components. To prove that the dynamical components of the breathers decay exponentially for large $\mathbf{n}$, we need to assume that the

[6] More precisely, it can be checked that the supremum norm which is proposed in that theory would have an sudden infinite variation when switching the perturbation at the anticontinuous limit for certain multibreather configurations as for example those shown figure 4, and thus cannot be used.

matrices $\mathbf{N}(\mathbf{q})$ and $\mathbf{P}(\mathbf{q})$ depend on the wavevector $\mathbf{q}$ as *analytic functions* in a band containing the real axis for each component of $\mathbf{q}$. This condition is equivalent to say that the coefficients of the Fourier series of these matrices which determine the atomic interactions, decays exponentially at long distance.

Now, to prove that the dynamical breather components indeed do decay exponentially, it is convenient to consider the linear equation fulfilled by the time derivative $\mathbf{\Phi}(t) = \dot{\mathbf{Y}}(t) = \{\phi_{\mathbf{n},\alpha}\}$ which is obtained by time differentiation of eq. 48

$$m\ddot{\phi}_{\mathbf{n},\alpha} + \sum_{\beta} \frac{\partial^2 V(\mathbf{y_n})}{\partial y_{\mathbf{n},\alpha} \partial y_{\mathbf{n},\beta}} \phi_{\mathbf{n},\beta} - k^2 (\mathcal{S}.\mathbf{\Phi}(t))_{\mathbf{n},\alpha} + k' \sum_{\mathbf{m},\beta} \frac{\partial^2 \mathbf{W}(\mathbf{Y}(t))}{\partial y_{\mathbf{n},\alpha} \partial y_{\mathbf{m},\beta}} \phi_{\mathbf{m},\beta} = 0 \qquad (61)$$

For large $\mathbf{n}$, this equation becomes asymptotic to the linear phonon equation where $\mathbf{Y}(t) = \mathbf{0}$ which is translationally invariant and we get

$$-mp^2\omega_b^2 \phi^p_{\mathbf{n},\alpha} + \sum_{\beta} \frac{\partial^2 V(\mathbf{0})}{\partial y_{\mathbf{n},\alpha} \partial y_{\mathbf{n},\beta}} \phi^p_{\mathbf{n},\beta} - k^2 \sum_{\mathbf{m},\beta} (\mathbf{S}_p)_{(\mathbf{n},\alpha),(\mathbf{m},\beta)} \phi^p_{\mathbf{m},\beta} + k' \sum_{\mathbf{m},\beta} \frac{\partial^2 \mathbf{W}(\mathbf{0})}{\partial y_{\mathbf{n},\alpha} \partial y_{\mathbf{m},\beta}} \phi^p_{\mathbf{m},\beta} = 0 \qquad (62)$$

$\mathbf{S}_p$ is defined by eq. 47. Since $p \neq 0$, $p\omega_b$ does not belong to the phonon spectrum and $\mathbf{S}_p(\mathbf{q}) = -\mathbf{P}(\mathbf{q}).(p^2\omega_b^2\mathbf{M} - \mathbf{N}(\mathbf{q})^{-1}.\mathbf{P}^t(\mathbf{q})$ is an analytic function of $\mathbf{q}$. Consequently, the coefficients $(\mathbf{S}_p)_{(\mathbf{n},\alpha),(\mathbf{m},\beta)}$ decay exponentially with the distance $|\mathbf{n} - \mathbf{m}|$.

Since at the anticontinuous limit, $p\omega_b$ has been assumed to be outside the phonon spectrum for all $p \neq 0$, this property remains true for (k, k') in a neighborhood of $(0, 0)$. Then, we expect in that neighborhood (no matter how the breather itself is extended!) that $\phi^p_{\mathbf{n},\alpha}$ decays exponentially to zero for large $\mathbf{n}$. The rate of the exponential decay should be faster at large order $|p|$. (see ref. [17]). The same behavior should be found for the breather distortion $\mathbf{y}^p_{\mathbf{n}}$ at frequency $p\omega_b$ as well as for the associated acoustic distortion $\mathbf{x}^p_{\mathbf{n}}$.

9.2 Linear stability

We now briefly examine the problem of the linear stability of a single breather solution close to the anticontinuous limit. Because of the existence of gapless acoustic phonons, this problem is more complex to analyse than in the simple case of optical breathers.

The linear stability of a solution $\mathbf{Y}(t), \mathbf{X}(t)$ is given the linearized equations (5) and (6). As we point out in subsection (4.2) and in ref. [6], it is convenient to embed this problem in the following eigenvalue problem

$$M_p \ddot{\eta}_{\mathbf{n},p,\alpha} + \sum_{\mathbf{m},q,\beta} N_{(\mathbf{n},p,\alpha),(\mathbf{m},q,\beta)} \cdot \eta_{\mathbf{m},q,\beta} + k \sum_{\mathbf{m},\beta} P_{(\mathbf{m},\beta),(\mathbf{n},p,\alpha)} \cdot \epsilon_{\mathbf{m},\beta} = E \eta_{\mathbf{n},p,\alpha} \tag{63}$$

$$m \ddot{\epsilon}_{\mathbf{n},\alpha} + \sum_{\beta} \frac{\partial^2 V(\mathbf{y_n})}{\partial y_{\mathbf{n},\alpha} \partial y_{\mathbf{n},\beta}} \epsilon_{\mathbf{n},\beta} + k \sum_{\mathbf{m},p,\beta} P_{(\mathbf{n},\alpha),(\mathbf{m},p,\beta)} \cdot \eta_{\mathbf{m},p,\beta} + k' \sum_{\mathbf{m},\beta} \frac{\partial^2 \mathbf{W}(\mathbf{Y})}{\partial y_{\mathbf{n},\alpha}, \partial y_{\mathbf{m},\beta}} \epsilon_{\mathbf{m},\beta} = E \epsilon_{\mathbf{n},\alpha} \tag{64}$$

The linear stability is determined by the solutions of this equation for $E = 0$. Since the second equation (64) has time periodic and time reversible coefficients, we can define the symplectic Floquet matrix $\mathbf{F}_E$, which relates linearly $\{\eta_{\mathbf{n},p,\alpha}(t_b)\}, \{\dot{\eta}_{\mathbf{n},p,\alpha}(t_b)\}, \{\epsilon_{\mathbf{n},\alpha}(t_b)\}, \{\dot{\epsilon}_{\mathbf{n},\alpha}(t_b)\}$ to the initial conditions $\{\eta_{\mathbf{n},p,\alpha}(0)\}, \{\dot{\eta}_{\mathbf{n},p,\alpha}(0)\}, \{\epsilon_{\mathbf{n},\alpha}(0)\}, \{\dot{\epsilon}_{\mathbf{n},\alpha}(0)\}$. For a linearly stable breather, the Floquet matrix $\mathbf{F}_0$ for $E = 0$, has all its eigenvalues on the unit circle.

Any eigensolution $\psi(t) = \{\eta_{\mathbf{n},p,\alpha}(t), \epsilon_{\mathbf{n},\alpha}(t)\}$ of eqs. 63 and 64 fulfills the Bloch-Floquet condition $\psi(t + t_b) = \psi(t) e^{i\theta}$ and the corresponding eigenvalue belongs to a band $E(\theta)$ which is 2π periodic and symmetric with respect to θ [6]. The intersections of these bands $E(\theta) = E$ determine the eigenvalues of the Floquet matrix $\mathbf{F}(E)$ which are on the unit circle. The Krein signature of this pair of eigenvalue is the opposite sign of the slope of the band intersection in the interval $]0, \pi[$ [6].

The evolution of the global band spectrum allows a better understanding of the instabilities which may occur. Then, it is useful to know first of all, this band structure at the beginning of the breather continuation when $k = k' = 0$. Then, the two equations (63) and (64) decouple and we get a collection of independent harmonic oscillators with frequencies $\omega(\mathbf{q})$ given by the eigenequation (11), and by the frequencies ω_μ of the linearized

anharmonic oscillators at their rest position defined from eq. 27. Each of these harmonic oscillators plus the anharmonic one, produces a family of bands which superpose.

The optical phonons of the molecule at the discrete set of frequencies ω_μ yield the series of bands $E^o_{\mu,n,\pm}(\theta) = m(\pm\omega_\mu^2 - (\theta + 2n\pi)^2/t_b^2)$ with n integer. They are "folded parabolae" over the interval $[-\pi, \pi]$ ("Brillouin zone"). Each of these band is degenerate $N-1$ times since there are $N-1$ oscillators at rest for a system of N unit cells.

The acoustic phonons yield continua of bands depending on the wave vector $\mathbf{q}$ which could be calculated in principle. The solution at $\mathbf{q} = 0$ determines the bands at the edge of this continuum which are $E^{a,\mathbf{q}=\mathbf{0}}_{n,\pm}(\theta) = -(\sum_p M_p)(\pm\theta + 2n\pi)^2/t_b^2$. They are d times degenerate. This is again a folded parabola, which for the branch $n = 0$ is tangent from below to the axis $E = 0$.

On top of that, there are nondegenerate bands corresponding to the spectrum of operator 30 for the single oscillating molecules calculated in subsection (4.2). There is again a band tangent to the axis $E = 0$ which is due to the phase mode. For illustration, we have shown an example figure 1 calculated for a real 3d potential.

With the superposition of three families of bands, the global band spectrum might become quite complex. Figure 5 shows a possible scheme for the simplest possible situation in one dimension where there is only two variables per unit cell. We distinguished two situations for the local anharmonic potential $V(\mathbf{y})$. In the first case the derivative of the energy of

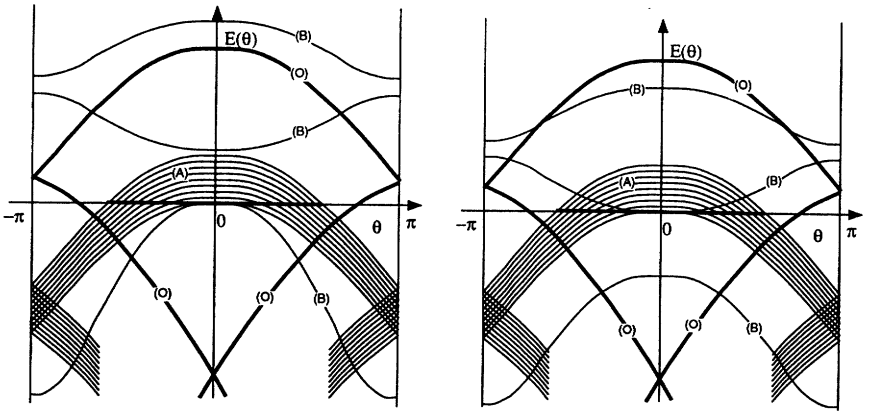

Fig. 5. – Scheme of the band structure at the anticontinuous limit for a hard potential (left) and for a soft potential (right). It is the superposition of bands associated with acoustic phonons denoted (A), with optical phonons (O) and of the single moving oscillator (B).

the local oscillation with respect to its frequency is positive (hard potential) and the second case where it is negative.

The eigenvalues $e^{\pm\theta_\sigma}$ of the Floquet matrix $\mathbf{F}_0$ at $E = 0$ which are on the unit circle are obtained as the intersection of the bands with the line $E = 0$. Then, the spectrum of the Floquet matrix consists of symmetric continuous arcs on the unit circle which corresponds to the harmonic modes. Among them, there at least two arcs which starts both from the eigenvalue 1 which corresponds to the gapless acoustic phonons and possibly several other arcs. There are also isolated eigenvalues on the unit circle which are degenerate and corresponds to the optical phonon mode. On top of these eigenvalues, there are also the Floquet eigenvalues corresponding to the Floquet matrix of the oscillating molecule described in subsection (4.2), If we have chosen initially a linearly stable solution, they are d pairs of eigenvalues on the unit circle but one of them corresponding to the phase mode is degenerate at 1.

Figure 6 shows the distribution of the Floquet eigenvalues on the unit circle which result from either case of fig. 5. It is clear that much information useful for understanding the breather instabilities is lost in that representation.

When k and k' are no more equal to zero, we have to understand from the initial band structure how it could evolve for producing breather instabilities that is some band intersections with the axis $E = 0$ are lost.

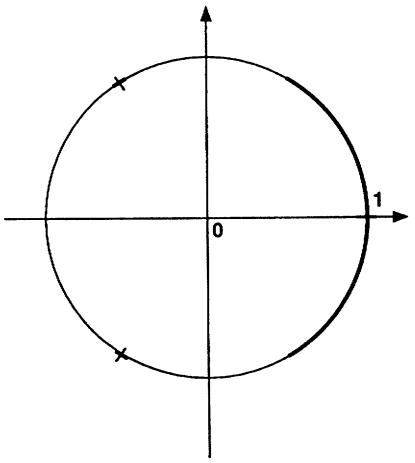

Fig. 6. – Distribution of the Floquet eigenvalues on the Unit circle for both examples of figure 5. There are two symmetric continuous arcs corresponding to the acoustic phonons, two symmetric isolated degenerate eigenvalues corresponding to the optical phonons and a twice degenerate eigenvalue at $+1$.

We do not treat the general case, but only a situation similar to those represented by figure 5.

In that case, the Floquet eigenvalues associated with the acoustic phonons form two symmetric arcs starting from 1 and they all have positive Krein signature. Concerning the degenerate Floquet eigenvalues associated with the optical phonon, it must be outside this arc if it has a negative Krein signature (but it could be inside if its Krein signature is positive). We can accept more complex situations with more phonon branches and more optical phonons but we assume that overlap between arcs of eigenvalues with different Krein signature do not occur.

Then, when k and k' varies, the band structure varies continuously as well as the breather solution. It keeps permanently $1 + d$ bands tangent to $E = 0$. One corresponds to the phase mode, and d bands corresponds to the translation modes of the crystal. Since the eigenvalues with different Krein signatures are separated by finite gaps, when k and k' are sufficiently small, no instability can result from the collision between these egeinvalues. There is only a risk of instability when two symmetric eigenvalues in the acoustic band collides at $+1$.

If such an event happens when k and k' vary, there is a bifurcation point at which there is a degenerate extra eigenvalue of the Floquet matrix at $+1$. Then, there is an extra eigenvalue at $E = 0$ in the spectrum of eqs. 63 and 64 at $\theta = 0$. The corresponding eigensolution is time periodic with period t_b and its component $\{\epsilon_{\mathbf{n},\alpha}\}$ is not zero (otherwise it would be necessarily a translation mode of the crystal). Then, the variables $\eta_{\mathbf{n},p,\alpha}$ can be eliminated from eq. 64 by using eq. 63 with the operator $\mathcal{S}$ defined in eq. 46. Since we proved that this operator is L^2, the linearized operator corresponding to eq. 48 has a spectrum which is close to those obtained at the anticontinuous limit when k and k' are zero. This operator at the anticontinuous limit has a discrete spectrum with isolated eigenvalues and only one zero eigenvalue corresponding to the phase mode. Then, provided k and k' remain small enough, there cannot exist an extra eigenvalue coming to zero. This prove the linear stability of the single breather in some neighborhood of the anticontinuous limit, when at this limit the eigenvalues of the Floquet matrix with different Krein signature are separated by gaps.

When there are arcs of eigenvalues with different Krein signature which are overlapping, we are in a situation where we could expect instabilities coming even for k and k' small. Indeed, for finite system where the continuous spectrum of the Floquet matrix is replaced by discrete eigenvalues, breathers should become unstable by Krein crunches occuring for k and k' both very close to 0. Actually, a similar situation where two

arcs on the unit circle of the Floquet spectrum overlap with opposite Krein signatures, was found for optical breathers and studied both numerically and analytically in [16]. We also expect finite size effects when there are acoustic phonons with cascades of thresholds corresponding to the occurence of weak instabilies followed by reentrant thresholds where the breather recovers its stability [7]. We also conjecture that the single breather in the *infinite system* recovers its linearly stable at least when k and k' are not too large.

The situation is quite different when an isolated eigenvalue associated with the moving oscillator, penetrates a continuous arc of the Floquet spectrum with a different Krein signature. Then, according to [16], there are also finite size effects but the instability persists for the infinite system.

The stability problem of multibreather should involve the effective action as we suggested in ref. [6] and will not be discussed here.

10. CONCLUDING REMARKS

A practical point which we did not discuss here is that the existence proof of breathers can be turned into efficient numerical calculations [9, 18].

The major result of this paper is that it confirms that the existence of breathers is universal. Indeed, it was often believed that the breathers described by simple models would be washed out in real systems. The argument was that their coupling with the many other degrees of freedom which were neglected, would produce their decay. This work contradicts this argument and proves that breathers may survive to complexity. Their existence does not depend on the number of parameters in the unit cell, nor on its periodicity. They could exist in crystal, amorphous material as well as in complex proteins. Their existence only depends on global conditions like their non resonance with the global phonon spectrum and their initial structural stability.

Breathers are objects which are highly stable at low temperature where they could survive over macroscopic times. Otherwise, we know from numerical investigations and theoretical approaches that they interact with phonons [20, 21] but roughly speaking, they have a physically reasonable

[7] These breather instabilities have no effect on their possible continuation since Krein crunches do not involve time reversible and time periodic eigenmodes.

long life time when their characteristic energy is much higher than the characteristic thermal energy.

We believe that it becomes now worthwhile to try to investigate some puzzling physical problems which have unsolved answers, concerning for example the hole burning [22], the effect of sonoluminescence [23] ... under the light of these new advances in breather theory.

Another important result we pointed out, is that breathers in real situations should be generally piezoactive. In ordinary crystal or in amorphous structures, the piezoactivity of breathers leads to crystal deformations which on average simply produces a crystal dilatation. This effect is not of major importance because it is well known when heating any material.

By contrast, piezoactive breathers could play a major role for understanding essential mechanisms of biology. One of the most puzzling challenges of biophysics is to understand how some proteins which are adsorbed on microtubules, move systematically in a determined direction [19]. These motions play an essential role in the living cells because these mobile units carry other attached proteins from the nucleus to other part of the cell where they are needed. At the scale of few nanometers, one should expect naively that the motion of the adsorbed proteins is a Brownian motion on the microtubule and thus is a random walk. Actually, precise observations shows that this motion is truly and essentially directive without almost not any randomness. It is also known that it is induced by the hydrolysis of ATP into ADP and in average, one hydrolysed ATP molecule makes the protein to move by one unit of the microtubule. The efficiency of this conversion is unexpectedly good and is close to one.

The sketch of a possible mechanism would be that an ATP molecule is captured by the moving protein at an appropriate and selective site and hydrolised. The energy which is released (about 0.3 eV) is much higher than the thermal energy at the temperature where the cells are living. Then, this energy can be captured as a (quantum) breather at a selective (resonant) location of the protein. This piezoactive breather should generate conformational changes of the protein producing finally after breather relaxation, one protein step. Such process repeated (randomly by ATP capture), should produce a perfectly directive walk along the microtubule.

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