Mobility and Reactivity of Discrete Breathers

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Abstract

Breathers may be mobile close to an instability threshold where the frequency of a pinning mode vanishes. The translation mode is a marginal mode that is a solution of the linearized (Hill) equation of the breather which grows linearly in time. In some cases, there are exact mobile breather solutions (found numerically), but these solutions have an infinitely extended tail which shows that the breather motion is nonradiative only when it moves (in equilibrium) with a particular phonon field.

More generally, at any instability threshold, there is a marginal mode. There are situations where excitations by marginal modes produce new type of behaviors such as the fission of a breather. We may also have fusion. This approach suggests that breathers (which can be viewed as cluster of phonons) may react by themself or one with each others as well as in chemistry for atoms and molecules, or in nuclear physics for nuclei.

1 Breathers by the Principle of Anticontinuity: Brief Review of Current Developments

The concept of nonlinear self-localization which is now emerging as ubiquitous in many highly nonlinear models, has an old historical origin. Although exact localized and time periodic solutions were already known for long in special integrable models such as the sine-Gordon [1] or the Ablowitz-Ladik equation [2], these solutions were nongeneric because they could not survive under most perturbations of the models. Landau was probably the first physicist who pioneered the concept of nonlinear localization when he found in 1933 that very generally a quantum electron strongly coupled to a polarizable medium could localize in a potential well created self-consistently and then form a polaron[3]. Actually, the concept of breathers appeared implicitly in many fields in physics but without its generality and terminology. As a unique example, it is straightforward to reinterpret in terms of breathers the old well-known Josephson Junction (JJ) effect between two superconductors. In the undamped limit, it is described by nothing but a Discrete Nonlinear Schrödinger equation with two sites only [4]. Then, the presence of a breather is just associated with a rotation of the phase difference between the two superconductors that is the JJ effect (The same ideas extend to JJ arrays [5,6]). Despite many precursive ideas, it was only in 1988 that Takeno and Sievers clearly suggested that intrinsically localized modes (*breathers*) in discrete anharmonic systems should be quite general and robust solutions existing in many nonlinear models [7] (for a review see [8]). We believe that the discovery of this concept is a major achievement in the recent years and should become the cornerstone of new important development in Nonlinear Physics with applications to a wide number of fields in Physics, Chemistry and Biology.

The first rigorous proof for the existence of breathers in a wide class of models was given later [9]. This proof was obtained by considering first a limit where the model reduces to a discrete array of uncoupled anharmonic oscillators. Then, breathers, corresponding to one oscillator moving freely, trivially exist and can be continued up to nonzero values of the coupling. This uncoupled limit which can be viewed as opposite to the integrable limit where the system is harmonic and spatially continuous, was named anti-integrable or anticontinuous [10,11]. This theory also holds with aperiodic lattices which may be random, it holds for coupled rotors (rotobreathers), for electrons coupled to anharmonic oscillators (polarobreathers) etc... [12].

The basic principle of these proofs can be extended for proving the existence of breathers in nonsymplectic models with dissipation [13,14]. It can be also extended to anharmonic models involving acoustic phonons for example to an extension of the d-dimensional version of the model described in [15] which couples linearly anharmonic optical variables with harmonic acoustic variables [16]. A different approach is proposed in [17] which introduces a new type of anticontinuous limit in diatomic FPU chains where the mass ratio between the light and heavy atoms goes to zero. It can be extended to higher dimensions [18]. These different extensions confirm how general is the concept of discrete breather, and that they can persist as exact solutions despite the increasing of the model complexity.

The same theory also predicts the existence of multibreather solutions obtained by continuation from the solutions where several oscillators move at the same frequency [12] and many of them are linearly stable. They can be clusters of a few number of breathers and then are still considered as breathers (e.g. 2-sites breathers). They can also be extended over arbitrary infinite clusters. When the cluster covers all the lattice sites, the multibreather becomes just an anharmonic plane waves. They have the property that they can transport energy by phase torsion over arbitrarily complex pattern called *rivers* [19]. Such solutions can persist even when the lattice is *random*. In that case, it is interesting to point out that these multibreather solution can transport energy while all the linear modes are completely localized and cannot transport any.

These existence proofs can be also turned into an efficient method for the practical calculation at the computer accuracy of any breather and multibreather solutions [20,21,5,19,22,15] in any model where they exist (including FPU chains).

At the anticontinuous limit, the breather quantization is trivial [12]. Within the standard action-angle representation, the operator corresponding to the action of the uncoupled anharmonic oscillator at site i, can be written as $I_i = a_i^+ a_i + 1/2$ using standard creation and annihilation boson operators a_i^+ and a_i (phonons). The anharmonicity of the oscillator is equivalent to the fact that $H(I_i)$ is not a linear function of I_i, that is the phonons are interacting. Then, a quantum breather just appears as a bonded (or antibonded) cluster of phonons at a given site and no phonon elsewhere.

When the oscillators are coupled with some coupling C which has to be small compared to the binding energies, a naive perturbation calculation shows that these bonded states of phonons should persist as narrow bands. Their band width is proportional to C^p where p is the number of phonons involved in the quantum breather. When p is large, this band width becomes negligible or equivalently the breather mass infinite [1]. Such behavior is indeed observed for the dimer problem [4] where the band width is replaced by a narrow splitting between two levels and also for the trimer [23]. If quantum breathers are narrow bands of bonded bosons, quantum polaron could be also viewed as narrow bands of a bonded state between an electron and many bosons. Quantum Bipolarons are the same but with 2 electrons in a singlet state bonded to a cluster of phonons.

2 Breather Mobility by Marginal Modes

It has been observed since several years that discrete breathers could be mobile in some models [24,25] (for a review see [8]) [2]. Mobile breathers for which the velocity can go to zero (or at least become small), can be studied by continuity

[1] This is the expected behavior when the classical breather is not mobile and when there is no accidental resonances between different breather structures with the same energy.

[2] Strictly speaking mobile breathers are no more time periodic solutions and they require a specific definition which we shall give later.

from the immobile breathers. This problem looks analogous to the study of mobile kinks which can be often well described with a collective coordinate as a massive particle moving in a periodic Peierls-Nabarro (PN) potential. Many numerically observed features for mobile breathers at low velocity, are indeed reminiscent of those of moving kinks and for that reason, it has been proposed that breather mobility could be also related to the vanishing of some Peierls-Nabarro barrier [26].

However, it turned out that this concept cannot be clearly defined [8] at least as a straightforward extension of the standard concept. The reason is that discrete breathers are not topologically conserved objects, and belong to a family of solutions the internal energy (and frequency) of which can vary continuously. If a PN energy barrier could be defined with a separatrix in the phase space, it could be believed that the breather could nevertheless overcome this barrier by tuning its frequency and releasing some of its internal energy. This point has been discussed in details [27]. This point of view is not totally convincing because it is not discussed whether this internal energy could be released.

We proposed a consistent definition for a PN barrier but for the action of the breather instead of its energy [28]. This approach could explain the formation of *intermediate* breathers which correspond to the intermediate extrema (*i.e.* not centered on a lattice site nor in the middle of a bond) of the Peierls-Nabarro action. They are indeed numerically observed in many cases and shall be discussed in another publication [29]. We shall see here that an *effective* PN barrier in energy could be nevertheless defined empirically.

Beside the vanishing of its PN energy barrier, the mobility of a kink is also related to the vanishing of the frequency of a pinning (or translation) mode. Breathers also may have internal modes which are spatially localized. Unlike the PN barrier, they have an unambiguous definition which hold as well for kinks. These modes can be used for testing the breather mobility. When a breather is (almost) freely mobile, there are small perturbations (namely kicks on the *translation mode*) which induce its motion at slow velocity. Unlike most linear perturbations which grows exponentially in time (for unstable modes) or remain bounded (for stable modes), such a perturbation grows linearly in time. We call such kind of perturbations *marginal modes*. In the limit of a zero velocity, the ideal breather trajectory tends to become a continuum of breather solutions (if it exists). As a result, there are also perturbations which remain bounded in time and thus do not put the breather into motion. They correspond to a breather pinning mode at zero frequency.

For investigating pinning and marginal modes, let us consider as an example, the standard discrete Klein-Gordon chain with Hamiltonian:

2.1 The Klein-Gordon Chain: Notations

$$\mathbf{H} = \sum_n \left(\frac{p_n^2}{2} + V(u_n) + \frac{C}{2}(u_{n+1} - u_n)^2 \right) \tag{1}$$

which consists of anharmonic oscillators with potential $V(x)$ and mass unity coupled by a nearest neighbor harmonic coupling with constant C. Let us consider a time reversible breather solution with period t_b of the dynamical equation

$$\ddot{u}_n + V'(u_n) - C(u_{n+1} + u_{n-1} - 2u_n) = 0. \tag{2}$$

The linearized equation which determines the "harmonic" modes of the breather

$$\ddot{\epsilon}_n + V''(u_n(t))\epsilon_n - C(\epsilon_{n+1} + \epsilon_{n-1} - 2\epsilon_n) = 0 \tag{3}$$

is similar to a linear discrete Schrödinger equation but with a time periodic potential $V''(u_n(t))$ with period t_b. This equation always has the trivial solution $\epsilon_n(t) = \dot{u}_n(t)$ (phase mode).

Integration over a period of time t_b of this equation determines the Floquet matrix $\mathbf{F}$ which relates linearly $\{\epsilon_n(t_b), \dot{\epsilon}_n(t_b)\} = \mathbf{F}\{\epsilon_n(0), \dot{\epsilon}_n(0)\}$ to its initial conditions $\{\epsilon_n(0), \dot{\epsilon}_n(0)\}$. This matrix is $2N \times 2N$ for a system with N sites. It is symplectic which implies that if λ is an eigenvalue then λ^*, $1/\lambda$ and $1/\lambda^*$ are also eigenvalues. The linear stability of the breather requires that there are N pairs of eigenvalues $\mathrm{e}^{\pm i\theta_\nu}$ are on the unit circle (we choose for convenience $0 \leq \theta \leq \pi$). The phase mode corresponds to a degenerate pair at $\theta = 0$. This Floquet matrix is also connected to the phonon scattering by the breather [30].

The linearly stable mode associated with an eigenvalue $\mathrm{e}^{i\theta_\nu}$ is time quasiperiodic and exhibits the series of frequencies $\omega_\nu = (\frac{\theta_\nu}{2\pi} + n)\omega_b$ with n integer. Thus, its frequency is defined modulo ω_b. We choose the determination $n = 0$ and $0 \leq \omega_\nu \leq \omega_b/2$.

2.2 Linear Stability and Spectrum of the Second Variation of the action

It has been shown in [12] that it is also convenient to study the equation

$$\ddot{\epsilon}_n + V''(u_n)\epsilon_n - C(\epsilon_{n+1} + \epsilon_{n-1} - 2\epsilon_n) = E\epsilon_n \tag{4}$$

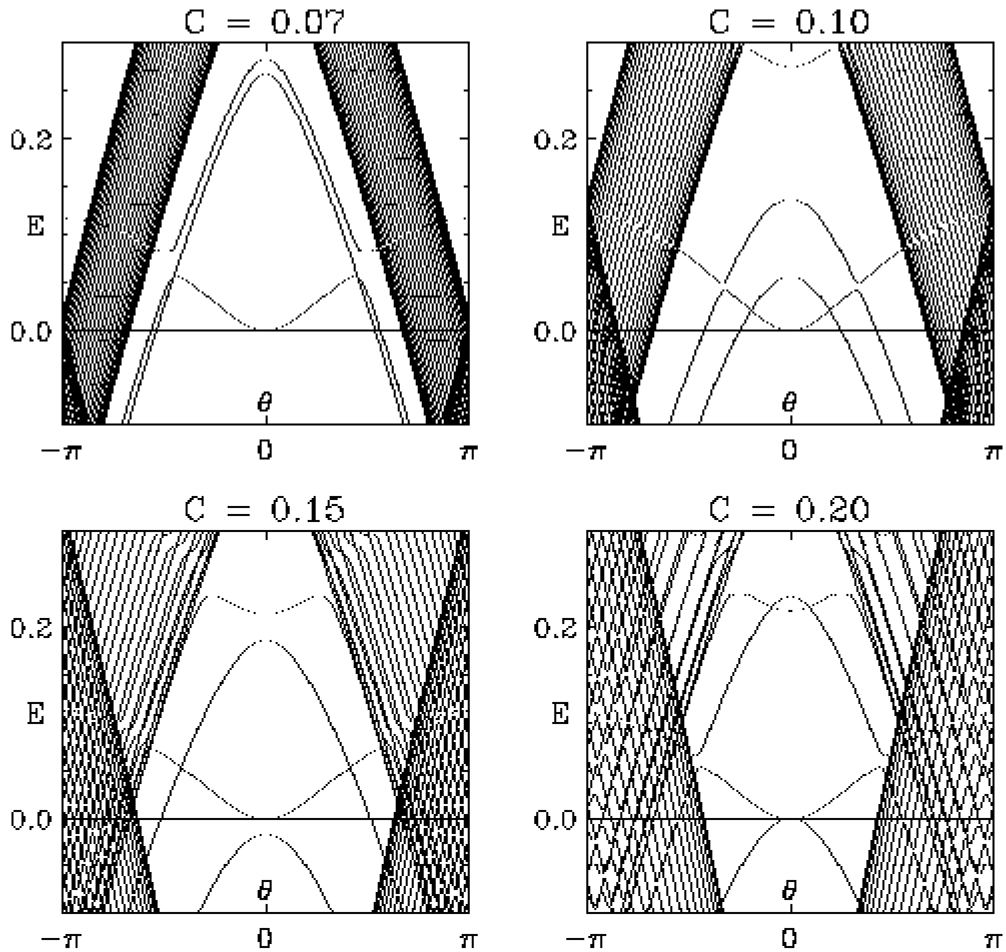

Fig. 1. Bands $E_\nu(\theta)$ defined by eqs.(4) and (5) calculated for the single breather at frequency $\omega_b = 0.75$ for the KG chain (1) with the Morse potential $V(x) = \frac{1}{2}(1 - \mathrm{e}^{-x})^2$ and $C = 0.07, 0.1, 0.15, 0.2$.

which allows one to explicit the Krein theory of bifurcations in simple terms and in addition, yields more informations. This is nothing but the eigenequation of the matrix of the second variation of the action expanded around the breather solution which by definition is one of its extrema. This is also the (full) Newton matrix involved in the breather continuation [12].

Let us make a brief review of its properties. The time periodicity of $V''(u_i(t))$ implies that the eigenvalues $E_\nu(\theta)$ of eq.(4) forms bands indiced by ν. They are 2π periodic and symmetric functions of the parameter θ defined modulo 2π and the corresponding eigenstates fulfills the Bloch condition

$$\epsilon_{\nu,n}(t + t_b, \theta) = \mathrm{e}^{i\theta t/t_b}\, \epsilon_{\nu,n}(t, \theta), \qquad n = 1, \ldots, N \tag{5}$$

(see fig.1 for an example of numerical calculation of the bands $E_\nu(\theta)$ of eq.(4)).

The eigenvalues $e^{\pm i\theta_\nu}$ of the Floquet matrix $\mathbf{F}$ which are on the unit circle, are determined by the set of intersections θ_ν of the bands $E_\nu(\theta)$ with the axis $E=0$. The Krein signature of a pair of conjugated eigenvalues $e^{\pm i\theta_\nu}$ is defined as[31]

$$\kappa(\theta_\nu) = \mathrm{sgn}\left(i\sum_n \epsilon_{\nu,n}\dot{\epsilon}^*_{\nu,n} - \epsilon^*_{\nu,n}\dot{\epsilon}_{\nu,n}\right) \tag{6}$$

which is a conserved quantity due to the symplecticity of the dynamics. According to the Krein theory, two pairs of eigenvalues $e^{\pm i\theta_\nu}$ and $e^{\pm i\theta_\mu}$ which collide on the unit circle may lead to an instability only if their signature is different. This criterion was reinterpreted in [12], where it has been shown that the Krein signature of the eigenvalues $e^{\pm i\theta_\nu}$ is the opposite sign of the slope $\mathrm{d}E_\nu(\theta)/\,\mathrm{d}\theta$ at $\theta=\theta_\nu$. Thus, it is clear that a bifurcation can occur only if the two eigenvalues belong to the same band (c.f. fig.2). As a consequence, the slopes of the band (or the Krein signatures) at θ_ν and θ_μ have to be different.

For a stable breather in a lattice with N sites, there are $N-1$ bands intersecting the axis $E=0$ and one corresponding to the phase mode which is tangent to this axis at $\theta=0$. When the system is infinite, there is a continuum of bands (see fig.1) which can be easily calculated because it corresponds to the spectrum of the system without breather ($u_i(t)\equiv 0$ and $V''(u_i(t))=\omega_0^2$) . There is at least one isolated band corresponding to the phase mode and possibly some other isolated bands which correspond to spatially exponentially localized modes.

2.3 Marginal Modes: Existence Proof

When the breather becomes linearly unstable, one of these bands $E_\nu(\theta)$ moves and looses its intersection (see fig.1 between $C=0.1$ and $C=0.15$, fig.2 and [12] for details). This appears on the unit circle as a collision between two eigenvalues θ_ν and θ_μ. At the bifurcation, we have three possible situations whether the curve is tangent to $E=0$ either at $\theta=0$, or at $\theta=\pi$ or at $\theta=\theta_0\neq 0$ or π (Krein crunch). The scheme on fig.2 shows an example for a Krein crunch.

Another important result which comes out readily from our band analysis is that the two eigenmodes associated with the eigenvalues $e^{i\theta_\nu}$ and $e^{i\theta'_\nu}$ are colinear at the bifurcation (see fig.2). Thus, the Floquet matrix $\mathbf{F}$ looses either one ($\theta=0$ or $\theta=\pi$) or two eigenvectors ($\theta=\theta_0\neq 0$ or π). As a consequence, the space generated by the eigenvectors of $\mathbf{F}$ is not the whole space. We show that the missing modes are just *marginal modes* which grows linearly in time.

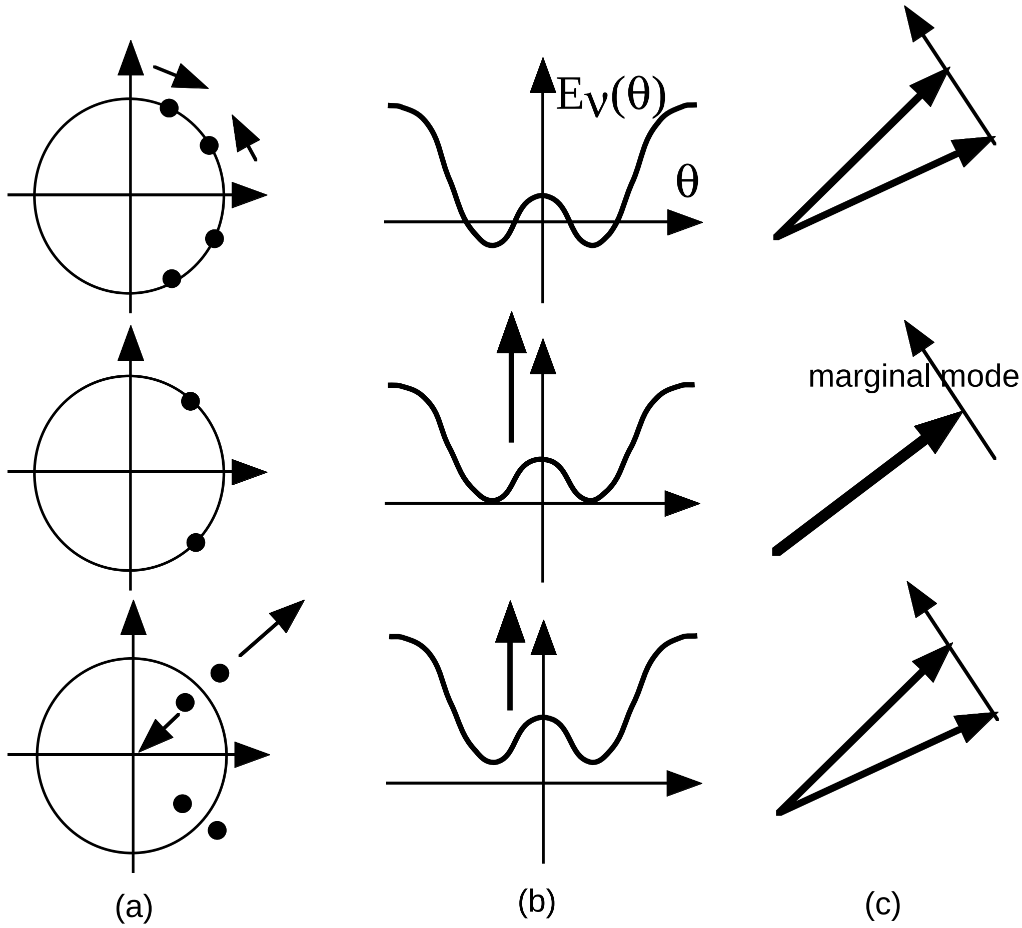

Fig. 2. Schemes showing as an example the evolution of four eigenvalues on the unit circle (a), the corresponding band shape of the matrix of the second variation of the action(b), the corresponding eigenvectors of the Floquet matrix for a Krein crunch before, at and after the bifurcation (c).

Let us prove that at each bifurcation where there is a curve $E_\nu(\theta)$ tangent from above (or from below) to the line $E = 0$ at $\theta = \theta_0$, eq.(3) exhibits a marginal mode.

The eigensolutions of eq.(4) associated with the eigenvalue $E_\nu(\theta)$ which fulfills the Bloch condition (5) can be written with the form $\epsilon_n^\nu(t,\theta) = \mathrm{e}^{i\theta t/t_b}\,\chi_n^\nu(t,\theta)$ where $\chi_n^\nu(t,\theta)$ is time periodic with period t_b. We assume for example that $E_\nu(\theta)$ is tangent to $E = 0$ from above. Then for $E > 0$ small enough, there are two values $\theta_1(E)$ and $\theta_2(E)$, such that

- $E_\nu(\theta_1) = E$ and $E_\nu(\theta_2) = E$
- $\lim_{E\to 0}\theta_1(E) = \theta_0$ and $\lim_{E\to 0}\theta_2(E) = \theta_0$.

Since the combination

$$\frac{\epsilon_n^\nu(t,\theta_1(E)) - \epsilon_n^\nu(t,\theta_2(E))}{\theta_1(E) - \theta_2(E)}$$

is also an eigensolution solution of eq.(4), it comes out that for $\theta = \theta_0$,

$$\frac{\partial \epsilon_n^\nu(t,\theta)}{\partial \theta} = \mathrm{e}^{i\theta t/t_b} \left(i\frac{t}{t_b}\chi_n^\nu(t,\theta) + \frac{\partial \chi_n^\nu(t,\theta)}{\partial \theta} \right) \tag{7}$$

is a solution of eq.(3) which diverges in time proportionally to t and thus is a marginal mode ($\partial \chi_n^\nu(t,\theta)/\partial\theta$ is time periodic with period t_b).

Thus, at the bifurcation, the Floquet matrix $\mathbf{F}$ exhibits a stable eigenmode $(\{\epsilon_n^\nu(0,\theta_0)\}, \{\dot{\epsilon}_n^\nu(0,\theta_0)\})$ for the eigenvalue $\mathrm{e}^{i\theta_0}$ associated with a marginal mode

$$\left(\{\frac{\partial \epsilon_n^\nu(0,\theta_0)}{\partial\theta}\}, \{\frac{\partial \dot{\epsilon}_n^\nu(0,\theta_0)}{\partial\theta}\} \right)$$

which grows linearly in time. When $\theta_0 \neq 0$ and π, the complex conjugate eigenvectors have the same properties. This property is associated with the fact that the 2×2 Floquet matrix restricted to the subspace determined by the two eigenvectors which becomes colinear at $\theta = \theta_0$, has degenerate eigenvalues but only one eigenvector and thus is not diagonalizable. The marginal mode is not uniquely defined. It could be combined arbitrarily with the associated eigenmode but this is just equivalent to change the origin of time.

As we pointed above, there is always a band $E_\nu(\theta)$ tangent at $E = 0$ for $\theta_0 = 0$. Equation (3) exhibits a phase mode ($\epsilon_n(t) = \dot{u}_n(t)$) for any breather solution and an associated marginal mode which diverges linearly in time. The latter can be also obtained directly by derivation of $u_n(t) = g_n(\omega_b t, \omega_b)$ with respect to ω_b and thus does not represent physically a real instability. Since an excitation of this mode produces a small change in the breather frequency, it is called growth mode.

2.4 Kicking a Breather

Turning back to the search of pinning mode and its associated marginal mode, we have to look for the breather bifurcations at $\theta_0 = 0$. A systematic analysis of the Floquet matrix of the breathers can be accurately and easily done numerically with the new methods developed in [20]. It yields many bifurcations and some of them are at $\theta = 0$. We just have to test numerically the effect of a breather perturbation in the direction of their marginal mode [3].

In the case of a spatially symmetric breather, the eigenmodes of eq.(4) are either spatially symmetric or antisymmetric. As a result the symmetric and

[3] Of course, perturbations in the direction of the growth mode, should not be excited for producing mobile breathers since its effect is just to change its frequency.

antisymmetric branches can intersect one with each other without interaction (*c.f.* fig.1). The pinning mode which corresponds to a small translation of the breather, has to break its spatial symmetry and should be searched as a spatially antisymmetric mode.

An example has been studied in detail for the KG model (1) with a double well potential $V(x) = \frac{1}{4}(x^2-1)^2$ [21]. More extensive numerical studies will be reported in [29]. We shortly recall the main findings and refer the reader to this reference for the illustrating figures.

For the double well potential and a single breather at frequency $\omega_b = 2\pi/6 < \omega_0 = \sqrt{2}$, the numerical analysis reveals that at $C = C_c \approx 0.5888$, there is a bifurcation at $\theta = 0$ concerning a spatially localized and antisymmetric eigenmode. There is a pair of isolated eigenvalues $\mathrm{e}^{\pm i\theta_1(C)}$ of the Floquet matrix $\mathbf{F}$ which go to unity for $C \to C_c$. The time reversibility of the breather solution implies that the pair of eigenvectors are complex conjugate and one is the image of the other by time reversibility. Thus they have the form $\mathbf{V}_\pm = (\{\delta_n(C)\}, \pm i\{\gamma_n(C)\})$ where the position component is real and the velocity component is purely imaginary. When $C \to C_c$, $\gamma_n(C_c) = 0$. The pinning mode $(\{\delta_n(C_c)\}, \{0\})$ only concerns breather perturbations on the position of the particles. The marginal mode which is both time antisymmetric and spatially antisymmetric, is obtained as the limit of the normalized vector $\lim_{C\to C_c} \hat{\mathbf{V}}(C)$ where $\hat{\mathbf{V}}(C) = \frac{\mathbf{V}(C)}{\|\mathbf{V}(C)\|_2}$ with $\mathbf{V}(C) = (\{0\}, \{\gamma_n(C)\})$. It contains only velocity components.

When a small initial perturbation with no component on the marginal mode is added to the breather, it does not move uniformly but only oscillates. On the opposite, it will move when the initial perturbation has a component on the marginal mode $\lambda\hat{\mathbf{V}}(C_c)$. The breather motion appears to be the most perfect (that is the most free of phonon radiation) when this perturbation is a pure marginal mode. A small perturbation $\lambda\hat{\mathbf{V}}(C_c)$ added to the initial conditions of the breather at $C = C_c$, grows linearly in time as expected. Actually, the breather moves slowly and the motion is uniform and persists over very long time and many lattice spacing with almost no energy dissipation. Let us emphasize that this breather mobility is not related to a large spatial extension of the breather as it is usually believed at least for mobile kinks.

This initial perturbation only concerns the initial velocity of the particles, which at $t = 0$ are zero for the unperturbed breather. Since $\hat{\mathbf{V}}(C_c)$ is normalized, the kinetic energy added to the breather by this initial kick is just $\frac{1}{2}\lambda^2$. It is found that the resulting velocity of this breather v is proportional to the amplitude λ. As a result, an effective mass m^* can be defined by the equality $\frac{1}{2}\lambda^2 = \frac{1}{2}m^* v^2$.

When C is close to but smaller than C_c, the breather does not move but

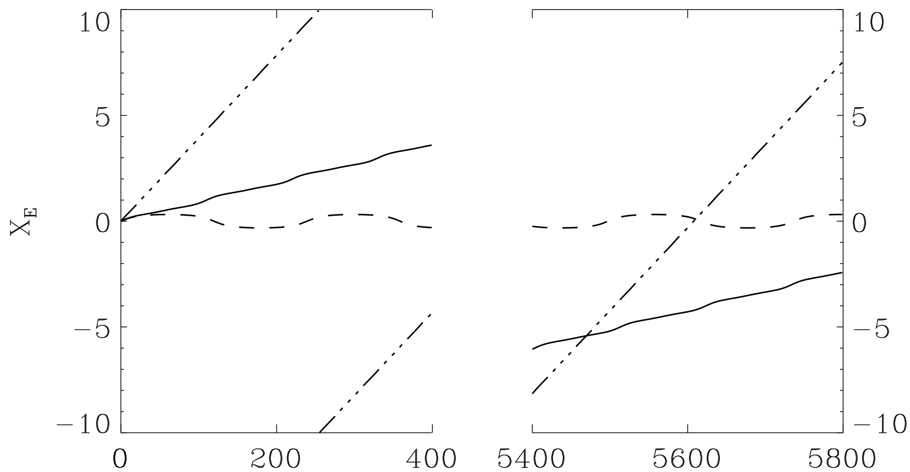

Fig. 3. Evolution of the center of energy (modulo 20) of a breather perturbed along its translation mode with various amplitudes: $\lambda < \lambda_c$ (dashed line), $\lambda \approx \lambda_c$ (full line) and $\lambda > \lambda_c$ (dash-triple dotted line). The on-site potential is the Morse potential, $C = 0.129$ and the frequency of the breather is $\omega_b = 0.80$. The unit of time is the period of the perturbed breather.

oscillates if the amplitude λ of the initial perturbation $\lambda \hat{\mathbf{V}}(C)$ is too small. This is not surprising because this perturbation does not correspond to a marginal mode but to an ordinary mode although its frequency is low. However, there exists a quite well-defined value $\lambda_c(C)$ such that when $\lambda > \lambda_c(C)$, the breather starts to move. Just beyond the threshold the motion is non uniform, similarly to a rotating pendulum near the separtrix. For larger kicks, the breather moves almost non-dissipatively over very long distances. An example is presented on fig.3 where a narrow linearly stable Morse breather is made mobile through a kick along its pinning mode. In some cases, the breather may dissipate phonon radiation and stop after some time. As a result, the determination of this mobility threshold cannot be determined with a high accuracy but its order of magnitude is nevertheless physically significant: $1/2\lambda_c^2$ can be interpreted as the *Peierls Nabarro energy barrier* which must be provided to move the breather. It is nonzero for $C < C_c$ and vanishes at $C = C_c$. It is undefined above (but could be defined from another intermediate breather [29]).

When C becomes larger than C_c, the breather is unstable and in principle a small perturbation $\lambda \hat{\mathbf{V}}(C)$ initially diverges exponentially. However, while the amplitude of this instability is weak enough, the mobility usually remains very good.

There are models for which the single breathers do not exhibit any instability threshold. Thus, no pinning mode can be found for example in the KG chain (1) with the quartic potential $V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$. All the numerical tests[21] we did by kicking these breathers by reasonably small initial perturbations, were unsuccessful to move the breathers even by few lattice spacings. However, a good mobility can be obtained when the breather frequency approaches the phonon band edge where the size of the breather diverges. This is not surprising because it is well-known that continuous models which do have exact propagating localized solutions (e.g. the Nonlinear Schrödinger equation), provides good approximation of the model in that limit.

In summary, highly mobile breather (which are not spatially very extended), may be found at the instability thresholds of the immobile breather. The numerical investigation of the spectrum and the eigenvalues of the Floquet matrix **F** allows one to discover systematically mobile breathers which are not spatially extended. The method has been applied successfully in various models including FPU chain and should work in principle for models in higher dimension. It has also been applied for finding *mobile* and *small* bipolarons in the Holstein-Hubbard model [32].

3 Exact Mobile Breathers: Loop Dynamics

Although the above method allows one to find breathers which moves with almost no energy dissipation, it is not clear whether there exists exact solutions corresponding to a moving breather.

Let us assume that we have an exact mobile breather solutions with frequency ω_b moving at the velocity v. After a time $T = 1/v$, the breather has moved by one lattice spacing, but since this time is generally incommensurate with the period $t_b = 2\pi/\omega_b$ of the breather, the breather phase has been rotated by an angle $\alpha = T\omega_b$ modulo 2π, incommensurate with 2π. After a time nT such that $nT\omega_b \approx 0$ modulo 2π, the breather returns to an almost identical configuration shifted by n lattice spacing. Therefore a moving breather should be viewed as a moving loop in the phase space. Its trajectory is the set of trajectories generated by the initial conditions with all possible phases. Such a dynamics can be described formally.

Considering a dynamical system with Hamiltonian $\mathbf{H}(\{p_i, u_i\})$ where u_i and p_i are conjugate variables and Hamilton equations

$$\dot{p}_i = -\frac{\partial \mathbf{H}}{\partial u_i} \qquad \dot{u}_i = \frac{\partial \mathbf{H}}{\partial p_i}. \tag{8}$$

We associate with this system, a dynamical system of loops $(\{p_{i,x}, u_{i,x}\})$ where the coordinates depends not only on i and but also on extra continuous variable

x on a 1-torus. For a given period t_b, we have

$$(\{p_{i,x+t_b}(y), u_{i,x+t_b}(y)\}) = (\{p_{i,x}(y), u_{i,x}(y)\}) \tag{9}$$

for any y which represents a (fictitious) time. Its trajectories extremalize the extended action

$$\mathcal{A} = \int dy \left(\int_0^{t_b} dx \sum_i p_{i,x}(y)(\frac{\partial u_{i,x}}{\partial x} + \frac{\partial u_{i,x}}{\partial y}) - \mathbf{H}(\{p_{i,x}(y), u_{i,x}(y)\}) \right) \tag{10}$$

which yields the extended Hamilton equations

$$\frac{\partial p_{i,x}}{\partial x} + \frac{\partial p_{i,x}}{\partial y} = -\frac{\partial \mathbf{H}}{\partial u_{i,x}}, \qquad \frac{\partial u_{i,x}}{\partial x} + \frac{\partial u_{i,x}}{\partial y} = \frac{\partial \mathbf{H}}{\partial p_{i,x}}. \tag{11}$$

The corresponding Hamiltonian for this loop dynamics is

$$\mathcal{H}_{\mathcal{L}}(y) = \int_0^{t_b} dx \left(\sum_i p_{i,x} \frac{\partial u_{i,x}}{\partial x} - \mathbf{H}(\{p_{i,x}, u_{i,x}\}) \right) \tag{12}$$

that is the action of the loop where $x = t$ is taken as the time in the initial model. For a solution of (11), this effective Hamiltonian is independent of the fictitious time y. Time periodic solutions with period t_b for the single time dynamics (and in particular the breathers) correspond to extrema of (12) and are fixed points for this loop dynamics.

An initial loop evolves in the phase space and in general if the system is mixing it will spread densely over the phase space (see fig.4). A mobile breather corresponds to a special solution of eqs.(11) which returns to an equivalent configuration apart a space translation. It fulfills the skew periodicity condition

$$(\{p_{i+1,x}(y+T), u_{i+1,x}(y+T)\}) = (\{p_{i,x}(y), u_{i,x}(y)\}) \tag{13}$$

Let us note that if $\{p_{i,x}(y), u_{i,x}(y)\}$ is a solution of eqs.(11), then for a and b arbitrary, $\{p_{i,ax+(1-b)y}(by+(1-a)x), u_{i,ax+(1-b)y}(by+(1-a)x)\}$ is also solution of the same equations. This change of variable does not change at all the corresponding set of real trajectories. However, our definition for the loop dynamics requires that the new solution be periodic with respect to x, which implies $b = 1$. The new period with respect to x which is t_b/a, can be arbitrary. In some sense, this is not surprising because strictly speaking the frequency of a mobile breather cannot be defined. However, it is reasonable that the loop

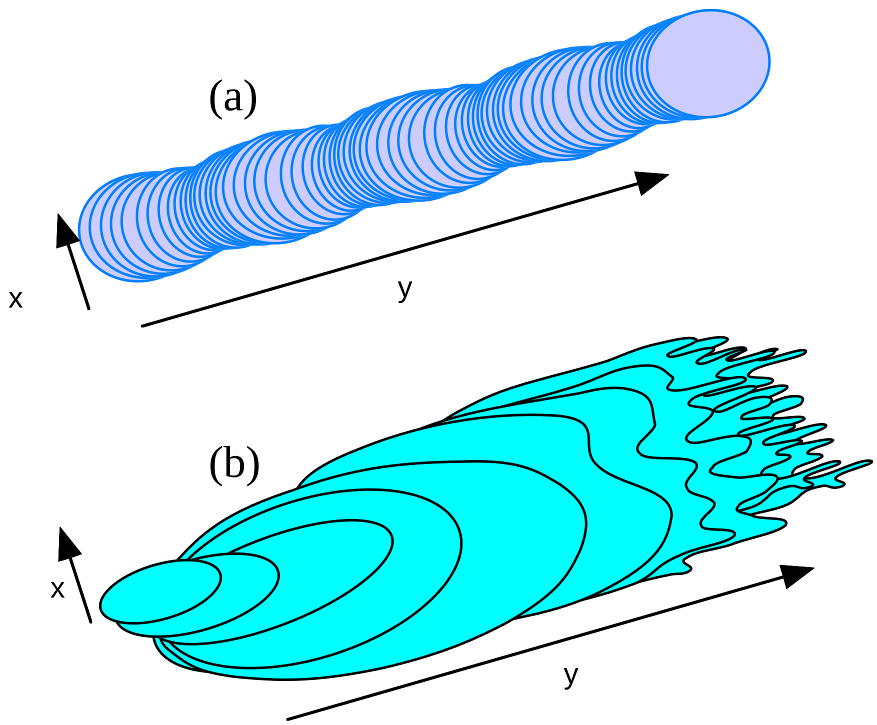

Fig. 4. Scheme of a Loop Dynamics : (a) represents the evolution in phase space of a loop which corresponds to an exact mobile breather. (b) the same for an arbitrary loop which *mixes* in the phase space

motion in the phase space be as slow as possible. a can be optimized for that and a possible criteria is that

$$\int_0^T dy \sum_i \left((\frac{\partial p_i}{\partial y})^2 + (\frac{\partial u_i}{\partial y})^2 \right)$$

be minimum.

If there is a solution of eqs.(11) which fulfills eq.(13) for a velocity $v = 1/T$, the energy of the initial loop $\mathbf{H}(\{p_{i,x}(0), u_{i,x}(0)\})$ has to be constant (i.e. independent of x). It is convenient to write this solution with hull functions $h_i(\xi, \eta, v)$ and $g_i(\xi, \eta, v)$ which are $2\pi-$periodic with respect to ξ, and 1-skew periodic with respect to η (that is $h_{i+1}(\xi, \eta + 1, v) = h_i(\xi, \eta, v)$ and $g_{i+1}(\xi, \eta + 1, v) = g_i(\xi, \eta, v)$). Then, we have $(\{p_{i,x}(y), u_{i,x}(y)\}) = (\{h_i(\omega_b x, vy, v), g_i(\omega_b x, vy, v)\})$. Eqs.(8) have a solution with the form

$$p_i(t) = h_i(\omega_b t + \alpha, v(t + \beta), v) \qquad u_i(t) = g_i(\omega_b t + \alpha, v(t + \beta), v) \quad (14)$$

where α and β are arbitrary phases.

Taking condition (13) into account, we have $h_n(\xi, \eta, v) = h_0(\xi, \eta - n, v)$ and

$g_n(\xi, \eta, v) = g_0(\xi, \eta - n, v)$ which shows that a unique pair of hull functions h_0, g_0 is sufficient for describing the whole breather motion. This new form turns out to be identical to those proposed by S. Flach for a mobile breather [33].

We have no mathematical proof that such exact solution could exist, but this problem could be approached numerically with the same methods as those used for calculating non time reversible multibreathers [19]. It consists in the application of a modified Newton method for finding fixed points of the Poincaré map $\mathbf{T}_L : \{p_{i,x}(0), u_{i,x}(0)\} \to \{p_{i+1,x}(T), u_{i+1,x}(T)\}$ defined by eqs.(11) where the period t_b and pseudoperiod T are given parameters. It is clear that as in [19], the Newton matrix is noninvertible at the fixed point (if any). We know however that these degeneracies are associated with the two arbitrary phases of eq.(14). As for nontime reversible breathers, this problem can be overcome by using a technique of singular value decomposition which in some sense, is equivalent to discard in the Newton matrix, the subspace associated with the two eigenvalues which are small. This method could converge to an exact solution, if one chooses as initial solution a good approximation of a mobile breather obtained by a marginal mode excitation. This general method has not yet been implemented.

We tested preliminarily the simplest case where T is an integer multiple of t_b. For that purpose, we just used the numerical program initially designed for non time reversible multibreather solutions [19] (a modified Newton method) with few line adaptations consisting in changing the time periodicity into the skew periodicity condition

$$\{p_i(t), u_i(t)\} = \{p_{i+1}(t+T), u_{i+1}(t+T)\}. \tag{15}$$

When a *good* approximate solution for a mobile breather can be obtained (by perturbation of an immobile breather with a translation mode), it can be used as trying solution for starting the Newton process. In that case, our program converges quite well to a *numerically exact* mobile breather solution at an accuracy, which is apparently only limited by the computer precision. This accuracy has been pushed till 10^{-21} (in quadruple precision) on the skew periodicity condition (15).

Figs.5 and 6 show two example of such solutions. The most striking feature is that the solution does not go exactly to zero far away from the center of the mobile breather but extends over the whole system whatever is its size. For the infinite system, this solution would likely spatially extend to infinity with a small amplitude oscillating tail. These mobile breather solutions look analogous to the nanopteron solutions [8] which are immobile breathers

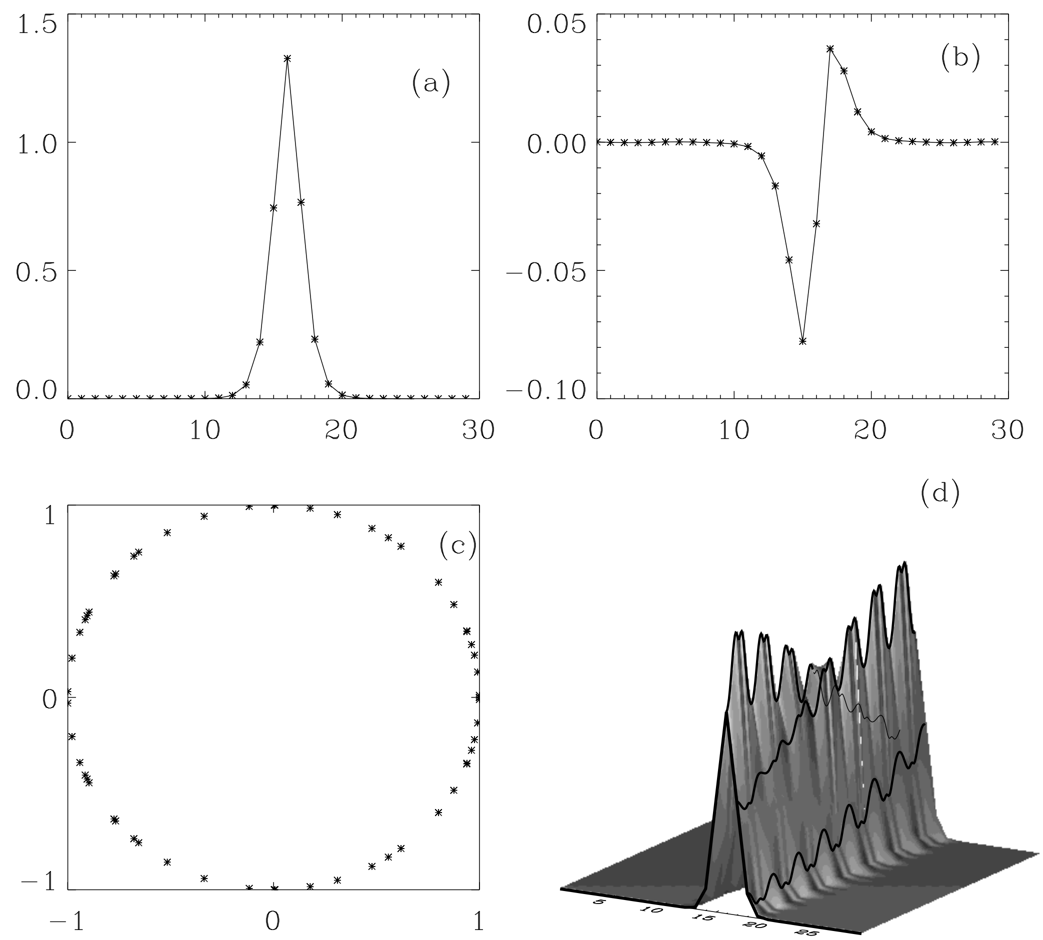

Fig. 5. Numerically Exact Mobile Breather obtained in the KG chain with the Morse potential at $C = 0.147$. The time needed to move over one lattice spacing is $T = 52.6$. Profiles of the initial positions (a) and velocities (b). (c) Distribution on the unit circle of the extended Floquet matrix $\mathbf{F}_e$. This solution is linearly stable. (d) Space-time representation of the energy density of the breather over one periode (there are 7 oscillations).

with an infinite phonon tail [4]. The extended Floquet matrix $\mathbf{F}_e$ defined as the derivative of the map $\{p_i(0), u_i(0)\} \rightarrow \{p_{i+1}(T), u_{i+1}(T)\}$ is numerically calculated and diagonalized in order to look at the stability of its fixed point.

In the case presented in fig.5, the mobile breather solution is linearly stable while in the second case where it is more discrete and moves slower, the mobile breather is slightly unstable. Further studies are necessary to explore these phenomena.

[4] They were named phonobreather in [12,20]. In some limit, their existence can be proved.

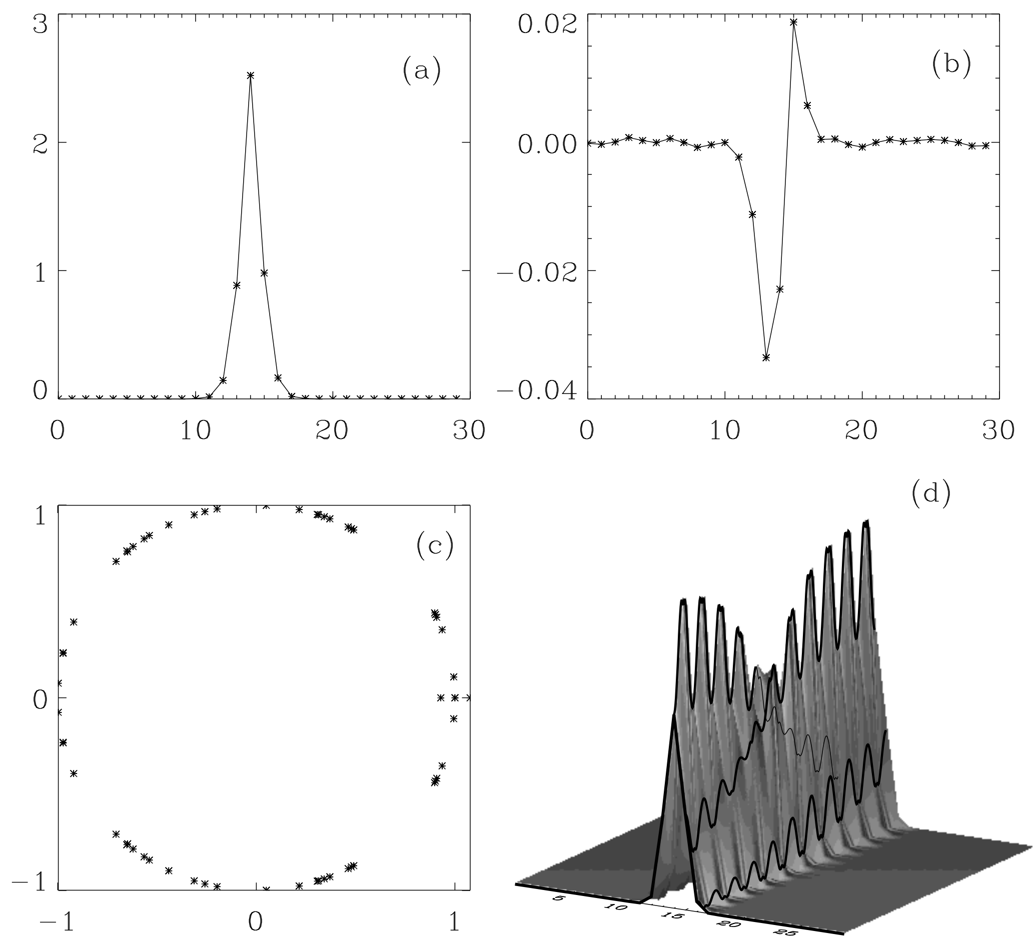

Fig. 6. Same as fig.5 but for $C = 0.1$, $T = 92$ and 10 internal oscillations over one period. Two eigenvalues are out of the unit circle and this exact solution is linearly unstable.

4 Breather Reactivity

As we found, in subsection 2.3, there are marginal modes at any breather bifurcation but only some marginal modes corresponding to bifurcations at $\theta = 0$ can be used for making a breather mobile. What is the effect on the breather of perturbations by marginal modes which are not associated with pinning modes? Since they diverge linearly in time, they start a slow transformation of the breather which is interesting to study at longer time. This transformation may exhibit complex transitory regimes not yet analyzed in general. In some cases, it exhibits a simpler behavior which can be easily interpreted.

For example, for a multibreather (2-breathers bonded state), we observed that its excitation by a marginal mode may produce a fission. The most typical case

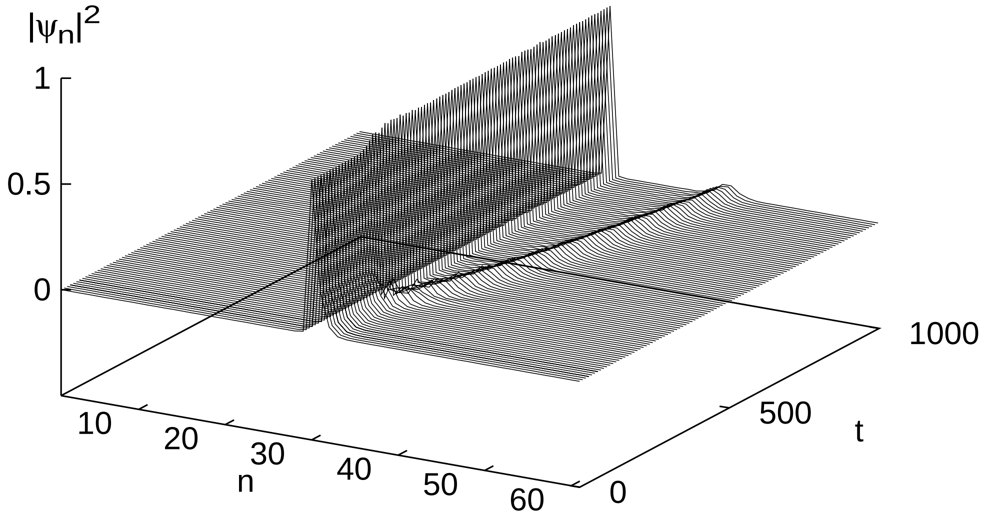

Fig. 7. Fission of a 2-breather state $\ldots \bullet\bullet\bullet\, 10 \bullet\bullet\bullet \ldots$ in the DNLS equation by a perturbation by the marginal mode at the instability threshold ($C = 0.065$, $\omega_b = (\sqrt{5}-1)/2$) (from ref.[22]).

we found (see fig. 7), was obtained in [22] for the DNLS equation

$$-C(\psi_{n+1} + \psi_{n-1} - 2\psi_n) - |\psi_n|^2\psi_n + \psi_n = i\dot{\psi}_n \tag{16}$$

for the 2-breather state denoted $\ldots \bullet\bullet\bullet\, 10 \bullet\bullet\bullet \ldots$ which is continued from the solution at the anticontinuous limit ($C = 0$) given by $\psi_0 = \sqrt{1+\omega_b}\, e^{i\omega_b t}$ (denoted 1), $\psi_1 = 1$ (denoted 0) and $\psi_i = 0$ for $i \neq 0$ and 1 (denoted $\bullet$). There is an instability threshold at $\theta = 0$ at which the marginal mode is time reversible. When at a given time, a small perturbation colinear to this marginal mode is added to the breather, this bonded state breaks after some time into "Big Brother" which stay immobile and "Little Brother" which is ejected and move quite far away before stopping. When C is smaller than its value at the 2-breather instability threshold, a critical perturbation (that is an energy threshold) is needed for having the fission (Peierls Nabarro energy barrier). Since the marginal mode is time reversible, the same behavior occurs when reversing time so that we get also an elastic collision scheme where running Little Brother collides elastically with Big Brother.

Let us show another example of perturbation by a marginal mode. Fig.8 shows the arguments of the Floquet matrix as a function of the coupling C for another 2-breather state which also consist of two identical breathers in anti-phase separated by 3 sites. The lattice is a KG chain with the Lennard-Jones on-site potential $V(x) = \frac{1}{72}(1 + (1+x)^{-12} - 2(1+x)^{-6})$. This configuration is linearly stable for small coupling but a Krein bifurcation occurs at $C \approx 0.105$ (the circle on Fig.8).

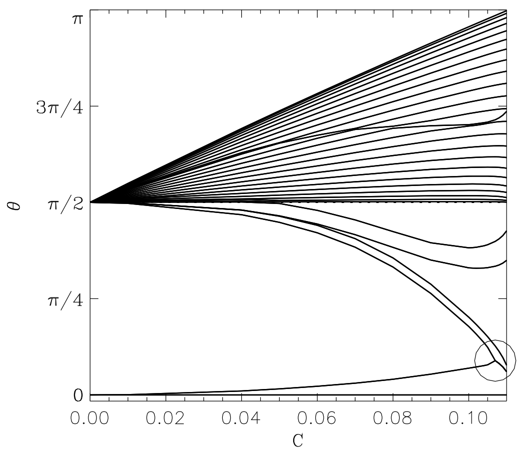

Fig. 8. Arguments θ of the eigenvalues of the Floquet matrix $\mathbf{F}$ versus the coupling C for the 2-breather $\ldots 00 - 1000100 \ldots$ at $\omega_b = 0.8$ of the KG chain with the Lennard-Jones potential.

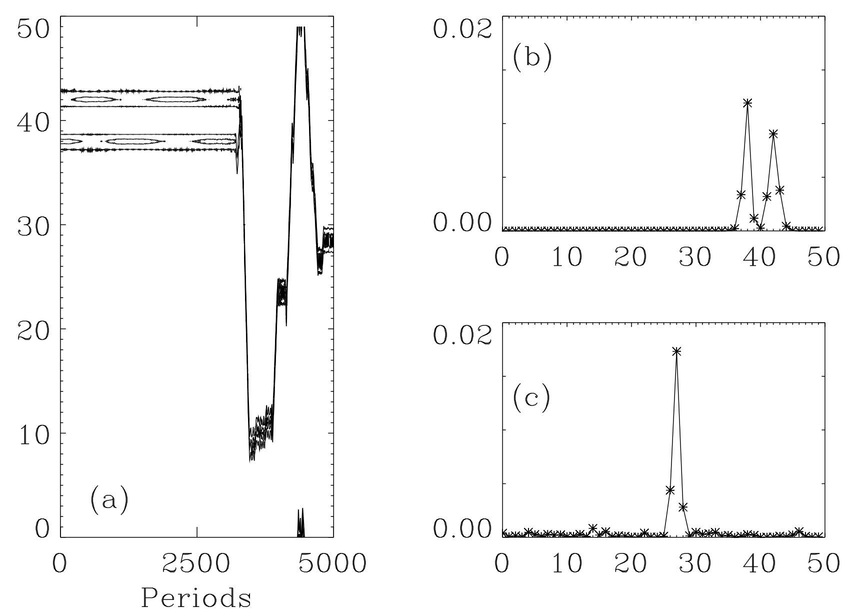

Fig. 9. Fusion associated with the marginal mode of the Krein bifurcation shown on fig.8. The norm of the perturbation is $\lambda \approx 10^{-2}$. (a) is a contour plot of the energy density versus time, (b) and (c) show the initial and final energy density.

A small excitation of this 2-breather by the associated marginal mode leads, after a long time (about 3000 Periods of the unperturbed breathers, see fig.9a) to a sudden fusion of the excitations. The resulting breather contains 75% of the total energy and is mobile. Its erratic motion is due to the radiation emited during the fusion.

These numerical studies are currently developed.

5 Concluding Remarks

In summary, we have shown the existence of a marginal mode growing linearly in time at any instability threshold. The existence of such a mode is a necessary condition (although not sufficient) for having a highly mobile breather and this condition is *not* necessarily related to large spatial breather extension as often believed. This criteria provides a systematic numerical method for testing breather mobility and then for finding easily in many models, spatially narrow breathers which are well mobile.

In addition, an improved Newton method allows to find numerically "exact" mobile breathers with an accuracy only limited by the computer precision. Actually, these mobile solutions have an infinite tail as the nanopterons which suggests that generally a strictly localized breather cannot propagate without radiating energy (but in some case this radiation can be extremely weak).

The marginal modes, appearing at any instability threshold, do not necessarily correspond to breather mobility. We found examples where excitation by a marginal mode produces the fission of a two breather bonded state. There are also examples where two colliding breathers merge into a bigger one (*i.e.* a breather fusion). Let us also quote that the inelastic interaction of weak amplitude phonons with breathers discovered in [30], can be viewed as a breather spallation.

Our studies presented here or in the related references, concerns classical models. However, this series of phenomena are reminiscent of chemical or nuclear reactions. This should not be surprising when thinking about the quantized version of these phenomena. Breathers are bonded (or antibonded) clusters ("molecules" or "nuclei") of n interacting particles which are bosons (physically, these bosons are "phonons"). Their classical stability depends on the breather amplitude or frequency, that is in the quantum representation of the number of bosons bonded together. Thus, depending on the model we may have stable quantum breathers for some values of n and unstable ones for other values. Actually, in translationally invariant models, these breathers form bands but their effective mass may be very high when they are not mobile. If this breather gets a high mobility, its effective mass should drop drastically [5] . It is also not surprising that these molecule could react with a

[5] We already numerically observed this phenomena for the quantized bipolarons of the Holstein-Hubbard model [32].

chemistry which of course highly depends on the choice of the boson interactions that is on the anharmonic potentials of the model.

Finally, let us note that arrays of very resistive Josephson junction (which can be modeled by the DNLS equation) are likely the simplest systems where these ideas on breather propagation and reactivity could be developed and tested experimentally almost directly.

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