

Breather initial profiles in chains of weakly coupled anharmonic oscillators

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Abstract

A systematic correlation between the initial profile of discrete breathers and their frequency is described. The context is that of a very weakly harmonically coupled chain of softly anharmonic oscillators. The results are structurally stable, that is, robust under changes of the on-site potential and are illustrated numerically for several standard choices. A precise genericity theorem for the results is proved.

1 Introduction

Chains of coupled anharmonic oscillators have many applications in condensed matter and biophysics as simple one-dimensional models of crystals or biomolecules. Of particular interest are the so-called “breather” solutions supported by such chains, that is, oscillatory solutions which are periodic in time and exponentially localized in space [1]. The simplest possible class of models, where all the oscillators are identical, with one degree of freedom, and nearest neighbours are coupled by identical Hooke’s law springs has been widely studied in this context. The equation of motion for the position $q_n(t)$ of the n -th oscillator ($n \in \mathbb{Z}$) is

$$\ddot{q}_n - \alpha(q_{n+1} - 2q_n + q_{n-1}) + V'(q_n) = 0 \quad (1)$$

where α is the spring constant and V is the anharmonic substrate potential, which we choose to normalize so that $V'(0) = 0$ and $V''(0) = 1$. MacKay and Aubry have proved the existence of breathers in the weak coupling (small α) regime of this system [2]. They noted that in the limit $\alpha \rightarrow 0$, system (1) supports a one-site breather, call it $\mathbf{q}_0 = (q_n)_{n \in \mathbb{Z}}$, where one site ($n = 0$ say) oscillates with period T while all the others remain stationary at 0. Using an implicit function theorem argument they proved existence of a constant period

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continuation \mathbf{q}_α of this breather away from $\alpha = 0$ provided α remains sufficiently small and $T \notin 2\pi\mathbb{Z}^+$.

Having established the existence of these breathers, the question remains: what do they look like? Of course, this problem has been intensively studied, and several efficient numerical schemes have been devised [3, 4]. The purpose of this note is to point out that significant, systematic qualitative information about breathers in weakly coupled chains can be obtained from the initial *direction* of continuation of one-site breathers,

$$\mathbf{q}'_0 := \left. \frac{\partial \mathbf{q}_\alpha}{\partial \alpha} \right|_{\alpha=0}. \quad (2)$$

Specifically, the small α behaviour of breathers can be determined by approximating the curve \mathbf{q}_α by its tangent line at $\alpha = 0$, that is

$$\mathbf{q}_\alpha = \mathbf{q}_0 + \alpha \mathbf{q}'_0 + o(\alpha). \quad (3)$$

Note that equation (3) is a precise mathematical statement, following directly from the MacKay-Aubry theorem, not a formal expansion. This allows one to make a systematic study of the frequency dependence of breather initial profiles for several on-site potentials. The results show a generic behaviour of alternating frequency bands of two qualitatively different types of breather, which we call “in-phase breathers” and “anti-phase breathers”. We go on to prove that this alternating behaviour is generic in a precise sense.

2 The direction of continuation of one-site breathers

In the following we will assume that $V : \mathbb{R} \rightarrow \mathbb{R}$ is twice continuously differentiable and has a normalized stable equilibrium point at 0 ($V'(0) = 0$, $V''(0) = 1$). Consider the equation of motion for a particle moving in such a potential,

$$\ddot{x} + V'(x) = 0 \quad (4)$$

with $\dot{x}(0) = 0$. Provided $|x(0)|$ is small enough, $x(t)$ must be a periodic oscillation. All the potentials we consider will be softly anharmonic with classical frequency spectrum $(0, 1)$.

Let $x_T(t)$ denote the solution of (4) with period $T > 2\pi$ and $x(0) > 0$ which has even time-reversal symmetry, $x_T(-t) \equiv x_T(t)$. From this we may construct a 1-site breather solution of system (1) with $\alpha = 0$, call it \mathbf{q}_0 :

$$q_{n,0}(t) = \begin{cases} x_T(t) & n = 0 \\ 0 & n \neq 0. \end{cases} \quad (5)$$

The MacKay-Aubry theorem establishes the existence of a continuation \mathbf{q}_α of this solution away from $\alpha = 0$ in a suitable function space, defined as follows.

Definition 1 For any $n \in \mathbb{N}$, let $C_{T,n}^+$ denote the space of n times continuously differentiable mappings $\mathbb{R} \rightarrow \mathbb{R}$ which are T -periodic and have even time reversal symmetry. Note that $C_{T,n}^+$ is a Banach space when equipped with the uniform C^n norm:

$$|q|_n := \sup_{t \in \mathbb{R}} \{|q(t)|, |\dot{q}(t)|, \dots, |q^{(n)}(t)|\}.$$

Definition 2 For any $n \in \mathbb{N}$,

$$\Omega_{T,n}^+ := \{\mathbf{q} : \mathbb{Z} \rightarrow C_{T,n}^+ \text{ such that } \|\mathbf{q}\|_n < \infty\}$$

where

$$\|\mathbf{q}\|_n := \sup_{m \in \mathbb{Z}} |q_m|_n.$$

Note that $(\Omega_{T,n}^+, \|\cdot\|_n)$ is also a Banach space.

The required function space is $\Omega_{T,2}^+$. By construction, $\mathbf{q}_0 \in \Omega_{T,2}^+$ and is exponentially spatially localized.

Theorem 3 (MacKay-Aubry) *If $T \notin 2\pi\mathbb{Z}$ there exists $\epsilon > 0$ such that for all $\alpha \in [0, \epsilon)$ there is a unique continuous family $\mathbf{q}_\alpha \in \Omega_{T,2}^+$ of solutions of system (1) at coupling α with \mathbf{q}_0 as defined in (5). These solutions are exponentially localized in space and the map $[0, \epsilon) \rightarrow \Omega_{T,2}^+$ given by $\alpha \mapsto \mathbf{q}_\alpha$ is C^1 .*

The idea of the proof is to define a C^1 mapping $F : \Omega_{T,2}^+ \oplus \mathbb{R} \rightarrow \Omega_{T,0}^+$,

$$F(\mathbf{q}, \alpha)_m = \ddot{q}_m - \alpha(q_{m+1} - 2q_m + q_{m-1}) + V'(q_m), \quad (6)$$

so that $F(\mathbf{q}, \alpha) = 0$ if and only if \mathbf{q} is an even T -periodic solution of system (1). In particular, $F(\mathbf{q}_0, 0) = 0$ by construction. Using $T \notin 2\pi\mathbb{Z}^+$ and anharmonicity of V , one can show that the partial derivative of F with respect to \mathbf{q} at $(\mathbf{q}_0, 0)$, $DF_{q_0} : \Omega_{T,2}^+ \rightarrow \Omega_{T,0}^+$, is invertible (DF_{q_0} is injective with $(DF_{q_0})^{-1}$ bounded). Hence the implicit function theorem [6] applies and local existence and uniqueness of the C^1 family \mathbf{q}_α satisfying

$$F(\mathbf{q}_\alpha, \alpha) = 0 \quad (7)$$

are assured. Persistence of exponential localization is proved as a separate step.

The object of interest in this paper is $\mathbf{q}'_0 \in \Omega_{T,2}^+$, the tangent vector to the curve \mathbf{q}_α at $\alpha = 0$. This may be constructed by implicit differentiation of (7) with respect to α at $\alpha = 0$:

$$DF_{q_0} \mathbf{q}'_0 + \left. \frac{\partial F}{\partial \alpha} \right|_{(\mathbf{q}_0, 0)} = 0 \quad \Rightarrow \quad \mathbf{q}'_0 = -(DF_{q_0})^{-1} \left. \frac{\partial F}{\partial \alpha} \right|_{(\mathbf{q}_0, 0)}. \quad (8)$$

Both DF_{q_0} and $\partial F / \partial \alpha|_{(q_0, 0)}$ are easily computed from (5,6). Evaluating the right hand side of (8) to find $\mathbf{q}'_0 = \chi \in \Omega_{T,2}^+$ is then equivalent to solving the following infinite decoupled set of ODEs for $\{\chi_m \in C_{T,2}^+ : m \in \mathbb{Z}\}$:

$$\ddot{\chi}_0 + V''(x_T)\chi_0 = -2x_T \quad (9)$$

$$\ddot{\chi}_m + \chi_m = x_T \quad |m| = 1 \quad (10)$$

$$\ddot{\chi}_m + \chi_m = 0 \quad |m| > 1. \quad (11)$$

Recalling that $T \notin 2\pi\mathbb{Z}^+$ (so $\cos \notin C_{T,2}^+$) one sees from (11) that $\chi_m \equiv 0$ for $|m| > 1$. So one need only solve the linear boundary value problems (9,10) with $\dot{\chi}_m(0) = 0$, $\chi_m(T) = \chi_m(0)$

for $m = 0, 1$ (clearly $\chi_{-1} \equiv \chi_1$), coupled to the nonlinear driver equation (4) for x_T . This is a numerically trivial task.

Having computed the initial value of the tangent vector, we may approximate the breather initial profile for small α using (3):

$$q_{m,\alpha}(0) = \begin{cases} x_T(0) + \alpha\chi_0(0) + o(\alpha) & m = 0 \\ \alpha\chi_1(0) + o(\alpha) & |m| = 1 \\ o(\alpha) & |m| > 1. \end{cases} \quad (12)$$

So to first order in α , the continuation leaves all but the central ($m = 0$) and off-central ($m = \pm 1$) sites at the equilibrium position. The qualitative shape of the breather initial profile depends crucially on $\chi_1(0)$ (but not $\chi_0(0)$). If $\chi_1(0) > 0$, the continuation displaces the off-central sites from equilibrium in the same direction as the central site. The result is a hump shaped breather in which the central and off-central sites oscillate, roughly speaking, in phase (that is they attain their maxima and minima simultaneously). We shall call such breathers “in-phase breathers (IPBs).” If $\chi_1(0) < 0$, on the other hand, the off-central sites are displaced in the opposite direction from the central site, resulting in a sombrero shaped initial profile. In this case, the central and off-central sites oscillate, roughly speaking, in anti-phase (the central site attains its maximum when the off-central sites attain their minima, and vice-versa). We shall call such breathers “anti-phase breathers (APBs).” We shall find that for a generic substrate potential V , system (1) supports both IPBs and APBs, the type varying in bands as T increases through $(2\pi, \infty)$.

3 Numerical results

The results presented in this section were generated using a 4th order Runge-Kutta method with fixed time step $\delta t = 0.01$ to solve the driver equation (4) for x_T and the linear boundary value problems (9,10). The results obtained depend crucially on whether the substrate potential has reflexion symmetry about the equilibrium position.

The following phenomenologically standard asymmetric potentials were investigated:

$$\text{Morse: } V_M(x) = \frac{1}{2}(1 - e^{-x})^2 \quad (13)$$

$$\text{Lennard-Jones: } V_{LJ}(x) = \frac{1}{72} \left(\frac{1}{x^{12}} - \frac{2}{x^6} \right) \quad (14)$$

$$\text{Cubic: } V_C(x) = \frac{1}{2}x^2 - \frac{1}{3}x^3. \quad (15)$$

Note that, although even, V_{LJ} is asymmetric about its equilibrium position $x = 1$. Graphs of $\chi_0(0)$ and $\chi_1(0)$ against T for all these potentials are presented in figure 1.

Since χ_0 is always positive, continuation always proceeds initially by pulling the central oscillator further away from equilibrium as α increases. Note also that χ_0 remains bounded as $T \rightarrow \infty$ if the single oscillator solutions $x_T(t)$ remain bounded (V_C) but grows unbounded otherwise (V_M and V_{LJ}). In all cases it grows unbounded as $T \rightarrow 2\pi$.

From figure 1 we see that the sign of $\chi_1(0)$ changes as T increases, leading to the prediction of T -bands of IPBs and APBs, as explained in section 2. The sign changes

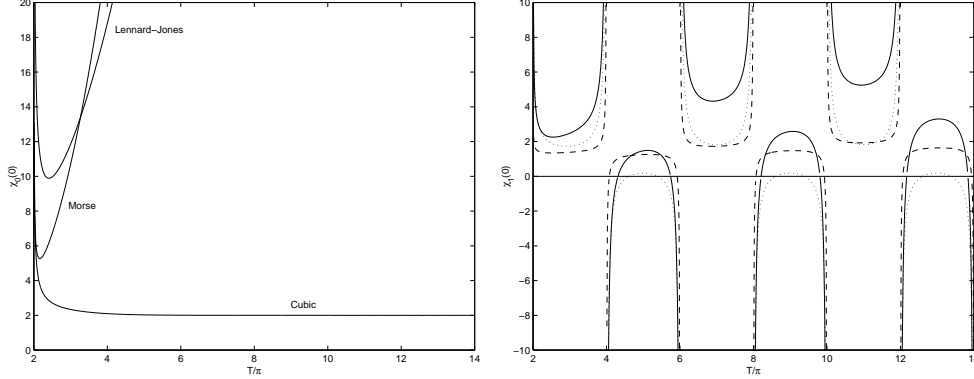


Figure 1: Graphs of $\chi_0(0)$ (left) and $\chi_1(0)$ (right) against T for various asymmetric on-site potentials (solid: Morse; dashed: Lennard-Jones; dotted: cubic).

are clearly associated with the vertical asymptotes of the graphs at each $T \in 2\pi\mathbb{Z}^+$. The presence of such asymptotes may be understood by using Green's function techniques to write down $\chi_1(t)$. First note that the particular integral for (10) with initial data $z(0) = \dot{z}(0) = 0$ is

$$z(t) = \int_0^t \sin(t-s)x_T(s) ds. \quad (16)$$

It follows from evenness of χ_1 that $\chi_1(t) = \chi_1(0)\cos t + z(t)$, and hence, applying the periodicity condition $\dot{\chi}_1(0) = \dot{\chi}_1(T)$, that

$$\chi_1(0) = \frac{1}{\sin T} \int_0^T \cos(T-t)x_T(t) dt. \quad (17)$$

Equation (17) shows that there is a vertical asymptote at $T = 2n\pi$, with a sign change in $\chi_1(0)$, unless

$$\int_0^{2n\pi} \cos t x_{2n\pi}(t) dt = 0, \quad (18)$$

that is, unless $x_{2n\pi}(t)$ has vanishing n -th Fourier coefficient. It might appear from (17) that there should also be asymptotes at $T = (2n+1)\pi$. This cannot be true since standard results on continuity of solutions of ODEs with respect to initial data imply that $\chi_1(0)$ is continuous for $T \notin 2\pi\mathbb{Z}^+$. In fact, a simple argument using periodicity and evenness of x_T demonstrates that

$$\int_0^{(2n+1)\pi} \cos t x_{(2n+1)\pi}(t) dt \equiv 0 \quad (19)$$

for all $n \in \mathbb{Z}^+$ and V . By contrast, we will prove in section 4 that (18) almost never holds (in a sense which will be made precise), so that the resonant periods $T = 2n\pi$ generically separate IPB bands from APB bands.

Turning to symmetric potentials, the following standard examples were investigated:

$$\text{Frenkel-Kontorova: } V_{FK}(x) = 1 - \cos x \quad (20)$$

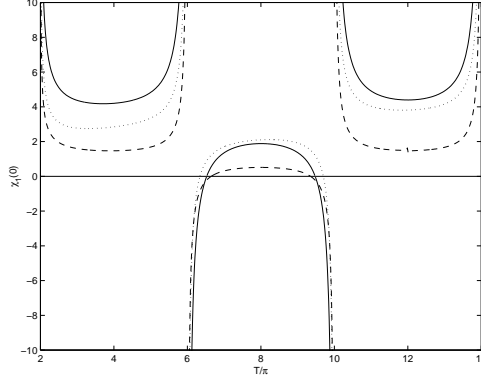


Figure 2: Graphs of $\chi_1(0)$ against T for various symmetric on-site potentials (solid: Frenkel-Kontorova; dashed: quartic; dotted: Gaussian).

$$\text{Quartic: } V_Q(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4 \quad (21)$$

$$\text{Gaussian: } V_G(x) = 1 - e^{-x^2/2} \quad (22)$$

The graphs of χ_0 display identical behaviour to that found for the asymmetric examples, and hence are not illustrated. The graphs of $\chi_1(0)$ against T , on the other hand, are strikingly different from the asymmetric case (see figure 2). In each case, vertical asymptotes are present at $T = 2n\pi$ only if n is an *even* positive integer. To explain this, note that evenness of V implies that $x_T(t)$ is $T/2$ antiperiodic, that is $x_T(t - T/2) \equiv -x_T(t)$, which in turn guarantees that equation (18) holds whenever n is odd. So alternating bands of IPBs and APBs occur for these potentials, but the alternation occurs half as often.

One universal feature of the graphs of χ_1 (independent of symmetry) is that $\chi_1 \rightarrow \infty$ as $T \rightarrow 2\pi$. This may easily be understood in the case where V is analytic (as in all our examples) by constructing a Linstedt expansion for $x_T(t)$ in the small amplitude regime [7].

4 Genericity of numerical results

The aim of this section is to prove the generic existence of a sign change in χ_1 as T crosses a resonance $T \in 2\pi\mathbb{Z}^+$. In particular, we will prove that, for a given n , the set of potentials on which (18) holds is negligibly small. To be precise, we will show that, for potentials in a certain Banach space \mathcal{P} , the subset of potentials on which (18) holds is locally a codimension 1 submanifold.

Definition 4 Let $\mathcal{P} = \{V : \mathbb{R} \rightarrow \mathbb{R} \text{ such that } V \text{ is } C^2 \text{ and } \|V\|_2 < \infty\}$ and $F : C_{T,2}^+ \oplus \mathcal{P} \rightarrow C_{T,0}^+$ be the mapping

$$F(q, V) = \ddot{q} + V'(q).$$

Note that F is a C^1 mapping between Banach spaces.

Definition 5 A potential $V \in \mathcal{P}$ is anharmonic at $q \in C_{T,2}^+$ if q is nonconstant, $F(q, V) = 0$, and $\ker DF_{(q,V)} = \{0\}$, where $DF_{(q,V)} : C_{T,2}^+ \rightarrow C_{T,0}^+$ denotes the partial derivative of F at (q, V) .

Clearly $F(q, V) = 0$ means that q is a solution of Newton's equation for motion in potential V . That injectivity of $DF_{(q,V)}$ is equivalent to the standard definition of anharmonicity in Hamiltonian mechanics is shown, for example, in the original proof of Theorem 3 [2]. For all the potentials we considered, V is anharmonic at $q = x_T \in C_{T,2}^+$ for all $T > 2\pi$.

Definition 6 A perturbation neighbourhood of $(q, V) \in C_{T,2}^+ \oplus \mathcal{P}$ is a pair (\mathcal{U}, f) where $\mathcal{U} \subset \mathcal{P}$ is an open set containing V , and $f : \mathcal{U} \rightarrow C_{T,2}^+$ is a C^1 map satisfying (a) every $W \in \mathcal{U}$ is anharmonic at $f(W)$ and (b) $f(V) = q$. Note that \mathcal{U} is trivially a Banach manifold.

Lemma 7 For any $V \in \mathcal{P}$ anharmonic at $q \in C_{T,2}^+$ there exists a perturbation neighbourhood (\mathcal{U}, f) of (q, V) . The function f is unique on sufficiently small \mathcal{U} .

Proof: Anharmonicity implies that $DF_{(q,V)}$ is injective, and hence the standard solvability criterion in linear ODE theory guarantees it is also surjective (see section 3.3.2 of [5] for details). The open mapping theorem then ensures boundedness of $DF_{(q,V)}^{-1}$. Hence $DF_{(q,V)}$ is invertible, and the implicit function theorem applied to F ensures existence of (\mathcal{U}, f) and local uniqueness of f . \square

Definition 8 For $T \in 2\pi\mathbb{Z}^+$, we shall say that $V \in \mathcal{P}$ is degenerate at $q \in C_{T,2}^+$ if V is anharmonic at q and

$$\int_0^T \cos t q(t) dt = 0.$$

Theorem 9 Let $T \in 2\pi\mathbb{Z}^+$, $V_0 \in \mathcal{P}$ be degenerate at $q_0 \in C_{T,2}^+$, and (\mathcal{U}, f) be a perturbation neighbourhood of (q_0, V_0) . The subset of \mathcal{U} on which degeneracy persists is a codimension 1 submanifold.

Proof: Consider the C^1 mapping $I : \mathcal{U} \rightarrow \mathbb{R}$ defined by

$$I(V) = \int_0^T \cos t [f(V)](t) dt$$

(I is C^1 since f is C^1). By the Regular Value Theorem (see appendix) the result follows if we establish that 0 is a regular value of I , or in other words that I is a submersion at every $V \in I^{-1}(0)$. Since $\ker DI_V$ is of finite codimension in $T_V\mathcal{U} = \mathcal{P}$ it splits and hence it suffices to show that $DI_V : \mathcal{P} \rightarrow \mathbb{R}$ is surjective for all $V \in I^{-1}(0)$.

Let $V \in I^{-1}(0)$, $q = f(V)$. For any $\delta V \in \mathcal{P}$, let $\delta q_{\delta V} = -[DF_{(q,V)}^{-1}(\delta V' \circ q)] \in C_{T,2}^+$. In other words $\delta q_{\delta V}$ is the unique even, T -periodic C^2 solution of

$$\delta \ddot{q}_{\delta V} + V''(q(t))\delta q_{\delta V} = -\delta V'(q(t)),$$

whose existence follows from anharmonicity of V at q (invertibility of $DF_{(q,V)}$ on $C_{T,0}^+$). With this notation,

$$DI_V(\delta V) = \int_0^T \cos t \delta q_{\delta V}(t) dt$$

and surjectivity of DI_V will follow if we exhibit $\delta V \in \mathcal{P}$ such that $DI_V(\delta V) \neq 0$. We construct such a δV in two steps.

For some $t_0 \in (0, T/2)$ and $\epsilon > 0$, let $b \in C_{T,2}^+$ be a non-negative function with $\text{supp } b \cap [0, T/2] = [t_0 - \epsilon, t_0 + \epsilon]$. Clearly

$$\int_0^T b(t) \cos t dt = 2 \int_0^{T/2} b(t) \cos t dt \neq 0$$

(where $T \in 2\pi\mathbb{Z}^+$ has been used) provided we choose $t_0 \notin \cos^{-1}(0)$ and ϵ sufficiently small. Since the critical points of $q(t)$ are isolated, we may also assume that q is invertible on $[t_0 - \epsilon, t_0 + \epsilon]$ with C^2 inverse $q^{-1} : [x_1, x_2] \rightarrow [t_0 - \epsilon, t_0 + \epsilon]$. By its construction the function g defined by

$$g(x) = \begin{cases} -[DF_{(q,V)}b] \circ q^{-1}(x) & x \in [x_1, x_2] \\ 0 & x \notin [x_1, x_2] \end{cases}$$

is in $C^0(\mathbb{R})$ (since DF maps to $C_{T,0}^+$). This allows us to construct a function $\delta\tilde{V}(x) \in C^1(\mathbb{R})$ such that $\delta q_{\delta\tilde{V}} = b$ as follows. For $x \in \text{ran}(q)$, $\delta\tilde{V}(x) = \int_0^x g(z) dz$ defines a C^1 function on $\text{ran}(q)$. Since $\delta q_{\delta\tilde{V}}$ is clearly independent of the behaviour of $\delta\tilde{V}$ outside $\text{ran}(q)$, we extend $\delta\tilde{V}$ to a C^1 function on \mathbb{R} with support contained in some compact set $K \supset \text{ran}(q)$.

We cannot immediately conclude that DI_V is surjective, since $\delta\tilde{V}$ is C^1 but not necessarily C^2 . However, using a density argument it is straightforward to find a $\delta V \in C^2$ close enough to $\delta\tilde{V}$ such that $DI_V(\delta V) \neq 0$ stills holds. More precisely, DI_V has a natural continuous extension, call it $\overline{DI_V}$ to C^1 . By construction $\delta\tilde{V}$ satisfies $\overline{DI_V}(\delta\tilde{V}) \neq 0$ and belongs to C_K^1 (the C^1 functions with support contained in K). Since C_K^2 is dense in C_K^1 , there exists a sequence $\delta V_m \in C_K^2 \subset \mathcal{P}$ converging (in C^1 norm) to $\delta\tilde{V}$, and by continuity $\overline{DI_V}(\delta V_m) \neq 0$ for all m sufficiently large. \square

In the above, we have chosen $\mathcal{P} = (C^2(\mathbb{R}), \|\cdot\|_2)$ as our space of potentials. This choice was made for the sake of clarity and notational simplicity – many other choices would work. In fact, all but two (V_{FK} and V_G) of the example potentials considered in section 3 lie, strictly speaking, outside \mathcal{P} , since they are unbounded. However, the analysis above can easily be adapted to deal with this: one simply replaces \mathcal{P} by the affine space $\mathcal{P}_V := \{W : \|W - V\|_2 < \infty\}$.

5 Comparison with tail behaviour

All our considerations so far have concerned the frequency dependence of breather initial profiles in the breather *core*, $|m| \leq 1$. It is interesting to compare these results with the profile behaviour in their *tails*, that is, for large $|m|$. Theorem 3 guarantees that breathers decay spatially exponentially fast, but gives no explicit information on the decay rate, or on sign correlations between neighbouring sites in the tail. Such information is obtainable,

at least heuristically, by means of the Fourier analytic approach of Flach [8]. We briefly recall this computation, adapted to our specific context.

Since the breather is spatially localized, time periodic with period $T = 2\pi/\omega$ and time reflexion symmetric, it has a Fourier series of the form

$$q_m(t) = \sum_{k=0}^{\infty} A_{m,k} \cos k\omega t, \quad (23)$$

with $A_{m,k} \rightarrow 0$ as $m \rightarrow \pm\infty$ for all k . Substituting (23) into (1) one obtains a nonlinear algebraic system for the coefficients $A_{m,k}$. Given the spatial decay criteria one expects these to be close, for large $|m|$ to solutions of the linearized algebraic system. This linearization decouples into a separate 2nd order linear difference equation for each mode k , namely

$$A_{m+1,k} - \left[2 + \frac{1 - k^2\omega^2}{\alpha} \right] A_{m,k} + A_{m-1,k} = 0, \quad (24)$$

whose general solution lies in the span of μ_k^m , μ_k^{-m} where μ_k is a root of

$$\mu^2 - \xi_k \mu + 1 = 0, \quad \xi_k := 2 + \frac{1 - k^2\omega^2}{\alpha} \quad (25)$$

with $|\mu_k| \leq 1$. The condition $A_{m,k} \rightarrow 0$ implies μ_k is real and $|\mu_k| < 1$. Hence the coefficient ξ_k in (25) must lie outside $[-2, 2]$ for all k , so $k\omega \notin [1, \sqrt{1+4\alpha}]$: every harmonic of ω must lie outside the phonon frequency band. Given this, all Fourier modes decay exponentially like $\mu_k^{-|m|}$.

In order to understand the tail behaviour, one must identify the dominant harmonic for large $|m|$, that is, the harmonic with slowest decay. Algebraically we seek that k , call it k_d say, which has $|\mu_k|$ closest to 1. Thinking of μ_k as the preimage $f^{-1}(\xi_k)$ where $f : (-1, 1) \setminus \{0\} \rightarrow \mathbb{R}$, $f(\mu) = \mu + \mu^{-1}$, one sees that this is the k for which $|\xi_k|$ is closest to 2. If $\xi_k > 2$ ($k\omega < 1$, below the phonon band), then

$$\alpha|\xi_k - 2| = 1 - (k\omega)^2, \quad (26)$$

while if $\xi_k < -2$ ($k\omega > \sqrt{1+4\alpha^2}$, above the phonon band), then

$$\alpha|\xi_k + 2| = (1 + 4\alpha) - (k\omega)^2. \quad (27)$$

Hence, the dominant harmonic is the one lying closest to the phonon band *in squared frequency space*. If $k_d\omega$ lies below the band, then $0 < \mu_{k_d} < 1$, and the tail has spatially uniform sign – the analogue for tail behaviour of an IPB. If $k_d\omega$ lies above the band, then $-1 < \mu_{k_d} < 0$ so the breather has an alternating tail, the tail analogue of an APB.

It is straightforward to partition the breather existence domain in (T, α) parameter space into IPB and APB subdomains according to this analysis, as shown in figure 3. In the period window $T \in [2\pi k, 2\pi(k+1)]$, one site breathers may be continued vertically from $\alpha = 0$ at most until the phonon band captures the $(k+1)$ th harmonic, $(k+1)\omega = \sqrt{1+4\alpha}$, giving the upper bounding curve

$$T_{ex}(\alpha) = 2\pi \frac{(k+1)}{\sqrt{1+4\alpha}}. \quad (28)$$

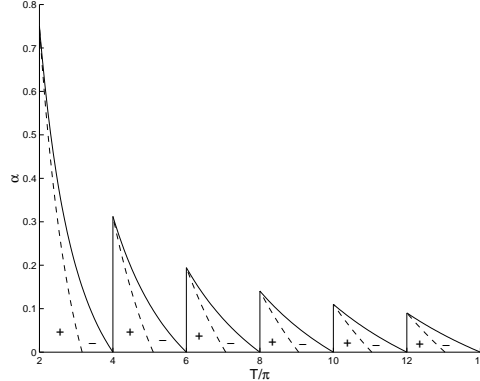


Figure 3: The breather existence domain for generic choice of substrate, partitioned into IPB-tail and APB-tail sectors, denoted + and – respectively.

This is the jagged upper curve depicted in figure 3. Within the existence domain below this curve, the transition between IPB and APB occurs where the pair $k\omega, (k+1)\omega$ straddling the phonon band become equidistant (in squared frequency space) from that band:

$$\begin{aligned}
 1 - k^2\omega^2 &= (k+1)^2\omega^2 - (1 + 4\alpha) \\
 \Rightarrow T_{trans}(\alpha) &= 2\pi\sqrt{\frac{k^2 + (k+1)^2}{2 + 4\alpha}}.
 \end{aligned}
 \tag{29}$$

These boundaries are depicted as dashed curves in figure 3. For fixed α , the transition with increasing T across each boundary is always from IPB to APB, denoted + and – respectively in the diagram.

Comparing this picture with figure 1 (which should be thought of as valid in a thin strip of the (T, α) plane containing the T axis) one sees that there will be many period intervals in which the core IPB/APB classification conflicts with the tail classification. In defence of our choice of terminology, based on the core behaviour, we note that breathers are interesting precisely because they are *localized* modes whose tails are exponentially small, so the core behaviour should be regarded as more significant than the tail behaviour. It is also worth noting two similarities between the core and tail analyses at small α . First, they are structurally robust, that is, qualitatively invariant under generic changes of the substrate potential. Second, the resonant frequencies $\omega = 1/n$ mark transitions between IPB and APB behaviour in both the core and tail senses.

Several caveats should be attached to the picture developed in this section. First, theorem 3 gives no guarantee that breathers really will exist in the whole domain depicted. Generically, it appears that they do, but there are Klein-Gordon-like systems with smaller existence domains [5]. Second, we have predicted the decay properties of a breather’s Fourier modes based on the linearized model. Numerically this approximation seems to work well most of the time. However, occasionally a few modes have anomalously slow spatial decay due to nonlinear corrections [8], so figure 3 may receive fine detail corrections. Third, it may be that some of the Fourier modes are wholly absent for symmetry reasons (e.g. V is symmetric). The picture is then modified substantially, in much the same way as the

core picture changes from figure 1 to figure 2. Finally, these results, while plausible, are heuristic. It would be interesting to seek a rigorous analytic underpinning for them.

6 Concluding remarks

In this paper, a systematic correlation between breather initial profiles and their frequencies was examined. Two types of breather were identified, called IPBs and APBs, based on sign correlations of the 3 core lattice sites. The numerical data suggest that generically these two types occur in alternating bands in the T parameter space ($T \in (2\pi, \infty)$), and that the resonant periods $T \in 2\pi\mathbb{Z}^+$ separate an IPB band from an APB band. The genericity of this behaviour was proved rigorously.

The distinction between IPBs and APBs, which does not appear to have attracted much attention in the literature, may have phenomenological implications in applications of the model (1). One reason for interest in discrete breathers (particularly continued one-site breathers) is that, because of their strong spatial localization, they typically require little energy to achieve large amplitude oscillations close to the centre. This makes them good candidates for “seeds” of mechanical breakdown of the network, the idea being that the central oscillation becomes so violent as to break the chain (a similar mechanism is postulated as a mechanism for DNA denaturation, for example [9]). One expects the central intersite springs to carry a larger proportion of the total breather energy for APBs than IPBs, making them more energy efficient seeds of mechanical breakdown. However, further detailed simulations of full lattice systems are required to test this hypothesis.

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Appendix

We recall some basic definitions and an elementary result of infinite dimensional differential topology, the Regular Value Theorem, which gives conditions under which the level set of a smooth function is guaranteed to be a manifold.

Definition 10 *We say that a closed subspace S of a complete topological vector space B splits if there exists another closed subspace C which is complementary to S , i.e. $C + S = B$ and $C \cap S = (0)$.*

Any finite dimensional subspace (necessarily closed) of a Banach space splits, as does any closed subspace of finite codimension.

Definition 11 A C^1 map $f : X \rightarrow Y$ between Banach manifolds is a submersion at $x \in X$ if $Df_x : T_x X \rightarrow T_{f(x)} Y$ is surjective and $\ker Df_x$ splits. A value $y \in Y$ is a regular value of f if f is a submersion for every $x \in f^{-1}(y)$.

Note that in the case that Y is finite dimensional then $\ker Df_x$ is of finite codimension in $T_x X$ and hence is guaranteed to split. In this case we need only verify that Df_x is surjective for f to be a submersion at x .

Theorem 12 (*The Regular Value Theorem*) Let $f : X \rightarrow Y$ be a C^1 map between Banach manifolds and $y \in Y$ be a regular value of f . Then $f^{-1}(y)$ is a submanifold of X with $T_x f^{-1}(y) \cong \ker Df_x$.

The proof follows from working in charts around x and $f(x)$ and applying the Implicit Function Theorem [10].

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