Breather initial profiles in chains of weakly coupled anharmonic oscillators

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Abstract
Qualitative information about breather initial profiles in the weak coupling limit of a chain of identical one-dimensional anharmonic oscillators is found by studying the linearized equations of motion at a one-site breather. In particular, information is found about how the breather initial profile depends on its period $T$. Numerical work shows two different kinds of breathers to exist and to occur in alternating $T$-bands. Genericity of certain aspects of the observed behaviour 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

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

where $\alpha$ 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 $\alpha$) regime of this system [2]. They noted that in the limit $\alpha \to 0$, system (1) supports a one-site breather, call it $q_0 = (q_n)_{n \in \mathbb{Z}}$, 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 $q_\alpha$ of this breather away from $\alpha = 0$ provided $\alpha$ 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? This question may be addressed by means of numerical analysis in several ways. One technique is to seek period $T$ solutions of a spatially truncated (i.e. $|n| \leq N < \infty$) version of (1) by searching for fixed points of the period $T$ Poincaré return map using, for example, a Newton-Raphson algorithm [3]. This method potentially allows the construction of breathers far from $\alpha = 0$, and can be used to determine the domain of existence of continued one-site breathers in the $(\alpha, T)$ parameter space (as applied by the authors to a non-standard discrete sine-Gordon system in [4]). This technique has its drawbacks, however. It is rather computationally expensive and there are subtleties concerning convergence of the Newton-Raphson method close to $\alpha = 0$ [3, 4]. On the other hand, if the weak coupling regime is of primary interest, then much useful information may be obtained from

$$q_0' := \left. \frac{\partial q_\alpha}{\partial \alpha} \right|_{\alpha=0},$$

(2)

the tangent vector at $\alpha = 0$ to the continuation curve $q_\alpha$. This vector may be calculated by solving a certain initial value problem for a set of 4 coupled second order ODEs, a numerically trivial task. The small $\alpha$ behaviour of breathers can then be determined by approximating the curve $q_\alpha$ by its tangent line at $\alpha = 0$, that is

$$q_\alpha = q_0 + \alpha q_0' + o(\alpha).$$

(3)

Since this method is so computationally cheap, it is easy to make a systematic study of the period dependence of breather initial profiles for a variety of substrate potentials. This paper presents such a study.

The paper is organized as follows. In section 2 we give a precise statement of the MacKay-Aubry existence theorem and reduce the calculation of $q_0'$ to numerically tractable form. In section 3 we present numerically generated graphs of the components of $q_0'$ against period $T$ for various choices of potential, and extract from them information about breather initial profiles in the small $\alpha$ regime. The results show a generic behaviour of alternating $T$-bands of two qualitatively different types of breather, which we call “in-phase breathers” and “anti-phase breathers”. In section 4 we prove that this alternating behaviour is generic in a precise sense, and examine the small $T$ limit analytically. Section 5 contains some concluding remarks.

2 The direction of continuation of one-site breathers

In the following we will assume that $V : \mathbb{R} \to \mathbb{R}$ 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,

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

(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 anharmonic with classical spectrum $(2\pi, \infty)$. Anharmonic
means that the period of oscillation varies nondegenerately with \(x(0) > 0\). The classical spectrum of \(V\) is the set of periods of the oscillations supported by \(V\).

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 \(q_0\):

\[
q_{n,0}(t) = \begin{cases} 
  x_T(t) & n = 0 \\
  0 & n \neq 0.
\end{cases}
\]  

The MacKay-Aubry theorem establishes the existence of a continuation \(q_\alpha\) of this solution away from \(\alpha = 0\) in a suitable function space, defined as follows.

**Definition 1** For any \(n \in \mathbb{N}\), let

\[C_{T,n}^+ := \text{the space of } n \text{ times continuously differentiable mappings } \mathbb{R} \to \mathbb{R} \text{ which are } T\text{-periodic and have even time reversal symmetry. Note that } C_{T,n}^+ \text{ is a Banach space when equipped with the uniform } C^n \text{ norm:} \]

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

**Definition 2** For any \(n \in \mathbb{N}\),

\[\Omega^+_{T,n} := \{q : \mathbb{Z} \to C_{T,n}^+ \text{ such that } ||q||_n < \infty\}\]

where

\[||q||_n := \sup_{m \in \mathbb{Z}} |q_m|_n.\]

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

The required function space is \(\Omega^+_{T,2}\). By construction, \(q_0 \in \Omega^+_{T,2}\) and is exponentially spatially localized.

**Theorem 3** (MacKay-Aubry) If \(T \not\in 2\pi\mathbb{Z}\) there exists \(\epsilon > 0\) such that for all \(\alpha \in [0, \epsilon)\) there is a unique continuous family \(q_\alpha \in \Omega^+_{T,2}\) of solutions of system (1) at coupling \(\alpha\) with \(q_0\) as defined in (3). These solutions are exponentially localized in space and the map \([0, \epsilon) \to \Omega^+_{T,2}\) given by \(\alpha \mapsto q_\alpha\) is \(C^1\).

The idea of the proof is to define a \(C^1\) mapping \(F : \Omega^+_{T,2} \oplus \mathbb{R} \to \Omega^+_{T,0}\),

\[
F(q, \alpha)_m = \ddot{q}_m - \alpha(q_{m+1} - 2q_m + q_{m-1}) + V'(q_m),
\]

so that \(F(q, \alpha) = 0\) if and only if \(q\) is an even \(T\)-periodic solution of system (1). In particular, \(F(q_0, 0) = 0\) by construction. Using \(T \not\in 2\pi\mathbb{Z}\) and anharmonicity of \(V\), one can show that the partial derivative of \(F\) with respect to \(q\) at \((q_0, 0)\), \(DF_{q_0} : \Omega^+_{T,2} \to \Omega^+_{T,0}\), is invertible \((DF_{q_0}\) is injective with \((DF_{q_0})^{-1}\) bounded). Hence the implicit function theorem applies and local existence and uniqueness of the \(C^1\) family \(q_\alpha\) satisfying

\[
F(q_\alpha, \alpha) = 0
\]
are assured. Persistence of exponential localization is proved as a separate step.

The object of interest in this paper is $q_0' \in \Omega^{+}_{2,T}$, the tangent vector to the curve $q_0$ at $\alpha = 0$. This may be constructed by implicit differentiation of (7) with respect to $\alpha$ at $\alpha = 0$:

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

Straightforward calculation shows that

$$[DF_{q_0} \chi]_m = \begin{cases} \ddot{x}_m + \chi_m & m \neq 0 \\ \ddot{x}_m + V''(x_T)\chi_m & m = 0 \end{cases}$$ (9)

for any $\chi \in \Omega^{+}_{2,T}$, and

$$\left( \frac{\partial F}{\partial \alpha} \right|_{(q_0,0)} \bigg|_m = \begin{cases} 2x_T & m = 0 \\ -x_T & |m| = 1 \\ 0 & |m| > 1. \end{cases}$$ (10)

So evaluating the right hand side of (8) to find $q_0' = \chi \in \Omega^{+}_{2,T}$ is equivalent to solving the following infinite decoupled set of ODEs for $\{\chi_m \in C^{+}_{2,T} : m \in \mathbb{Z}\}$:

$$\ddot{x}_0 + V''(x_T)\chi_0 = -2x_T$$ (11)
$$\ddot{x}_m + \chi_m = x_T$$ (12)
$$\ddot{x}_m + \chi_m = 0$$ (13)

Recalling that $T \notin 2\pi \mathbb{Z}^+$ (so $\cos \notin C^{+}_{2,T}$) one sees from (10) that $\chi_m \equiv 0$ for $|m| > 1$, so one need only compute $\chi_0$ and $\chi_1$ (clearly $\chi_{-1} \equiv \chi_1$).

In each case we must find the even $T$-periodic solution of an inhomogeneous 2nd order linear ODE. For $m = 0,1$ let $y_m(t)$ be the solution of the corresponding homogeneous equation with initial data $y_m(0) = 1$, $\dot{y}_m(0) = 0$, so

$$\ddot{y}_0 + V''(x_T)y_0 = 0$$ (14)
$$\ddot{y}_1 + y_1 = 0.$$ (15)

(Of course $y_1 = \cos$.) Similarly, let $z_m(t)$ denote the particular integral of the inhomogeneous equation with initial data $z_m(0) = \dot{z}_m(0) = 0$, so

$$\ddot{z}_0 + V''(x_T)z_0 = -2x_T$$ (16)
$$\ddot{z}_1 + z_1 = x_T.$$ (17)

Since $\chi_m(t)$ is even, it follows that $\chi_m(t) = \chi_m(0)y_m(t) + z_m(t)$, and $\chi_m(0)$ may be determined by applying either of the $T$-periodicity constraints

$$\chi_m(T) = \chi_m(0) \Rightarrow \chi_m(0) = \frac{z_m(T)}{1 - y_m(T)}$$ (18)
$$\ddot{\chi}_m(T) = \ddot{\chi}_m(0) \Rightarrow \chi_m(0) = -\frac{\dot{z}_m(T)}{y_m(T)}.$$ (19)
In either case, one sees that the tangent vector \( q'_0 \), and in particular its initial value \( q'_0(0) = (\ldots, 0, \chi_1(0), \chi_0(0), \chi_1(0), 0, 0, \ldots) \) can be constructed once the 4 initial value problems (14–17) are solved on \([0, T]\).

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

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

So to first order in \( \alpha \), 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).”

Sievers and Takeno have argued (without giving a rigorous mathematical proof) that breathers of the latter type are supported by certain oscillator chains with no substrate potential and anharmonic nearest neighbour coupling, but their existence in systems of type (1) does not seem to have attracted attention previously in the literature. This is surprising in light of the numerical results described in section 3. 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

Calculation of the constants \( \chi_0(0) \) and \( \chi_1(0) \) may be performed numerically by solving the initial value problems (14), (16) and (17) using some approximate ODE solver (recall the exact solution of (15) is known). The results presented in this section were generated using a 4th order Runge-Kutta method with fixed time step \( \delta t = 0.01 \). Each ODE requires the periodic oscillation \( x_T(t) \) as input. For most potentials this function must itself be generated by numerical solution of the oscillator equation (4), which might just as well be solved in parallel with (14,16,17), making 4 coupled 2nd order ODEs in all. Since the correct initial displacement \( x_T(0) \) for a given period \( T \) is not known in advance, the initial value problem is parametrized by initial displacement, \( T \) being determined from the approximate solution of (4) by counting sign changes of \( x_T(t) \) and linear interpolation.

The results obtained depend crucially on whether the substrate potential has reflexion symmetry about the equilibrium position.
3.1 Asymmetric potentials

The following asymmetric potentials were investigated:

\begin{align*}
\text{Morse: } V_M(x) &= \frac{1}{2}(1 - e^{-x})^2 \\
\text{Lennard-Jones: } V_{LJ}(x) &= \frac{1}{72} \left( \frac{1}{x^{12}} - \frac{2}{x^6} \right) \\
\text{Cubic: } V_C(x) &= \frac{1}{2}x^2 - \frac{1}{3}x^3.
\end{align*}

Note that the equilibrium position for $V_{LJ}(x)$ is $x = 1$ rather than $x = 0$, as we have been assuming so far. Hence, even though $V_{LJ}$ is even, it is still asymmetric, since it is not reflexion symmetric about $x = 1$. Graphs of $\chi_0(0)$ and $\chi_1(0)$ against $T$ for all these potentials are presented in figures 1 and 2 respectively.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Graphs of $\chi_0(0)$ against $T$ for various asymmetric substrate potentials.}
\end{figure}

Figure 1 illustrates a clear difference in the large $T$ behaviour of $\chi_0(0)$ between $V_C$ and the other two potentials $V_M$ and $V_{LJ}$. Namely $\chi_0(0)$ remains bounded as $T \to \infty$ for $V_C$, but grows unbounded for $V_M$ and $V_{LJ}$. This phenomenon appears to be linked to the large $T$ behaviour of the $T$ periodic oscillations $x_T(t)$. Due to the unstable equilibrium point of $V_C$ at $x = 1$, $x_T(t)$ tends to a bounded homoclinic orbit as $T \to \infty$ for this potential, and $\chi_0(0)$ is correspondingly bounded for large $T$. For $V_M$ and $V_{LJ}$ no such bounded homoclinic orbit exists: $x_T(0)$ is an unbounded function of $T$ and $\chi_0(0)$ is correspondingly unbounded as $T \to \infty$. In all cases, we note that $\chi_0(0) > 0$, so the continuation to $\alpha > 0$ displaces the central site further from equilibrium.
Figure 2: Graphs of $\chi_1(0)$ against $T$ for various asymmetric substrate potentials (solid: Morse; dashed: Lennard-Jones; dotted: cubic).

From figure 2 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 are clearly associated with the vertical asymptotes of the graphs at each $T \in 2\pi\mathbb{Z}^+$ (note that these do not conflict with the contents of section 2 since the existence proof for $q_\alpha$, and hence for $q_0$, breaks down when $T \in 2\pi\mathbb{Z}^+$). The presence of such asymptotes may be understood by using Green’s function techniques to write down $z_1(t)$, the solution of (17):

$$z_1(t) = \int_0^t \sin(t-s)x_T(s)\,ds. \quad (24)$$

Combining (24) with (19), and recalling that $y_1 = \cos$, yields a formula for $\chi_1(0)$,

$$\chi_1(0) = \frac{1}{\sin T} \int_0^T \cos(T-t)x_T(t)\,dt. \quad (25)$$

Equation (25) shows that there is a vertical asymptote at $T = 2n\pi$, with a sign change in $\chi_1(0)$, unless

$$\int_0^{2n\pi} \cos t \, x_{2n\pi}(t)\,dt = 0, \quad (26)$$

that is, unless $x_{2n\pi}(t)$ has vanishing $n$-th Fourier coefficient. It might appear from (25) that there should also be asymptotes at $T = (2n + 1)\pi$. Of course, 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

$$\int_0^{(2n+1)\pi} \cos t \, x_{(2n+1)\pi}(t)\,dt = 0 \quad (27)$$
for all $n \in \mathbb{Z}^+$ and $V$. By contrast, we will prove in section 4 that (26) 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.

### 3.2 Symmetric potentials

The following symmetric potentials were investigated:

- **Frenkel-Kontorova**: $V_{FK}(x) = 1 - \cos x$ \hspace{1cm} (28)
- **Quartic**: $V_Q(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4$ \hspace{1cm} (29)
- **Gaussian**: $V_G(x) = 1 - e^{-x^2/2}$ \hspace{1cm} (30)

The graphs in figure 3 show $\chi_0(0)$ against $T$ and closely resemble those of the previous section: $\chi_0(0)$ is bounded as $T \to \infty$ if $x_T$ tends to a bounded homoclinic orbit ($V_{FK}$ and $V_Q$), and unbounded if $x_T(0) \to \infty$ as $T \to \infty$ ($V_G$).

![Figure 3: Graphs of $\chi_0(0)$ against $T$ for various symmetric substrate potentials.](image)

Figure 3: Graphs of $\chi_0(0)$ against $T$ for various symmetric substrate potentials.

On the other hand, the graphs of $\chi_1(0)$ against $T$ (see figure 4) are strikingly different from the asymmetric case. In each case, vertical asymptotes are present at $T = 2n\pi$ only if $n$ is an even positive integer. If $n$ is odd, no asymptote is present. 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 (26) holds whenever $n$ is odd. The limit $\lim_{T \to 2n\pi} \chi_1(0)$ ($n$ odd) exists and may, in principle, be computed using L'Hospital’s rule with

$$\frac{d}{dT} z_1(T) = x_T(T) + \int_0^T [-\sin(T - t)x_T(t) + \cos(T - t)f'(T)y_0(t)] \, dt,$$

where $y_0$ is the solution of (14) as before and $f(T) := x_T(0)$. 

8
3.3 Almost symmetric potentials

For \( m = 1 \) equation (18) becomes

\[
\chi_1(0) = \frac{z_1(T)}{1 - \cos T}.
\]  

(32)

From this equation it is clear that the behaviour of \( \chi_1(0) \) as a function of \( T \) is largely determined by the zeroes of \( z_1(T) \). In particular, the sign of \( z_1(T) \) determines the sign of \( \chi_1(0) \). Figure 5 shows typical zero distributions for both asymmetric and symmetric potentials. It is interesting to note that no infinitesimal perturbation of the symmetric type distribution yields the asymmetric type distribution. Hence the dependence of \( \chi_1(0) \) on \( T \) for an almost symmetric potential must differ qualitatively from the typical asymmetric behaviour observed in section 3.1.

Asymmetric

\[
\begin{array}{cccccccccc}
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times \\
2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & T/\pi
\end{array}
\]

Symmetric

\[
\begin{array}{cccccccccc}
\times & \times & \times & \times & \times & \times & \times & \times & \times & \times \\
2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & T/\pi
\end{array}
\]

\( \times \) = simple zero, \( \otimes \) = double zero

Figure 5: Typical zero distributions of \( z_1(T) \) for asymmetric and symmetric substrates.
This observation motivates us to consider $z_1(T)$ for the following 1-parameter family of potentials:

$$V_\epsilon(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4 - \frac{\epsilon}{5}x^5. \quad (33)$$

The zeroes of $z_1(T)$ in a region of the $(T, \log \epsilon)$ plane are plotted in figure 6. In the symmetric limit ($\log \epsilon \to -\infty$), the typical symmetric type distribution is recovered, as expected. For a fixed but very small $\epsilon > 0$ (e.g. $\log \epsilon = -30$), the small $T$ oscillations $x_T(t)$ are pointwise essentially unchanged from the $\epsilon = 0$ case, and the distribution for small $T$ is numerically indistinguishable from the symmetric case. Only for large $T$ does the oscillation $x_T(t)$ detect the asymmetry of $V_\epsilon$, and a transition from symmetric to asymmetric behaviour occurs in the distribution. As $\epsilon$ is increased, the period at which this transition occurs becomes smaller and smaller, so that the transition “propagates” leftwards as seen in figure 6. For sufficiently large $\epsilon$ (e.g. $\log \epsilon > -3$) the transition is complete and the typical asymmetric distribution is recovered. These observations appear to be essentially independent of the asymmetric perturbation considered.

Figure 6: Zero distribution of $z_1(T)$ for the one parameter family of almost symmetric substrates $V_\epsilon(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4 - \frac{\epsilon}{5}x^5$.

4 Genericity of numerical results

The aim of this section is to explain some of the generic features observed in the numerical results of section 3. In particular we will consider the $T \to 2\pi^+$ behaviour of $\chi_1(0)$, and the generic presence of asymptotes at $T \in 2\pi\mathbb{Z}^+$.

4.1 The small period limit

The numerical data suggest that $\chi_1(0) \to +\infty$ as $T \to 2\pi^+$ for every potential $V$. We may confirm this prediction, at least in the case where $V$ is analytic (as is the case in all our
extract the asymptotic form of $z$ where all we need know about $y$ up to order $\epsilon$. Defining a rescaled time variable $s := \omega(\epsilon)t$ (so the solution is $s$-periodic with period $2\pi$) and dependent variable $y(s) := x(t)/\epsilon$ (so $y(0) = 1, y'(0) = 0$ for all $\epsilon$), we substitute the expansions

$$\omega(\epsilon) = a_0 + a_1\epsilon + a_2\epsilon^2 + \ldots$$

$$y(s) = y_0(s) + \epsilon y_1(s) + \epsilon^2 y_2(s) + \ldots$$

into (34) and Taylor expand $V(x)$ about $x = 0$. Grouping terms by order in $\epsilon$, this results in an infinite set of coupled ODEs for $\{y_n : n \in \mathbb{N}\}$, to be solved in turn ($n = 0, 1, 2, \ldots$) with initial data $y_0(0) = 1$, $y_0(0) = y_n(0) = 0$. Demanding that each $y_n(s)$ have period $2\pi$ then fixes the constants $a_0, a_1, a_2, \ldots$. For our purposes, it is sufficient to proceed only up to order $\epsilon^2$, whereupon one finds that

$$\omega(\epsilon) = 1 - A\epsilon^2 + O(\epsilon^3)$$

$$T(\epsilon) = 2\pi[1 + A\epsilon^2 + O(\epsilon^3)],$$

where $A = -V^{(4)}(0)/16 - (V^{(3)}(0))^2/12$ is positive for each of our examples (since they are all softly anharmonic, i.e. $T > 2\pi$). The

$$x_{T(\epsilon)}(t) = \epsilon \cos\omega(\epsilon)t + \epsilon^2 y_1(\omega(\epsilon)t) + \epsilon^3 y_2(\omega(\epsilon)t) + \ldots$$

where all we need know about $y_1, y_2, \ldots$ is that they are even with period $2\pi$. We can now extract the asymptotic form of $z_1(T(\epsilon))$ for small $\epsilon$:

$$z_1(T(\epsilon)) = \int_0^{T(\epsilon)} \sin(T(\epsilon) - t)x_{T(\epsilon)}(t) \, dt$$

$$= \frac{1}{\omega(\epsilon)} \int_0^{2\pi} \sin\left(\frac{2\pi - s}{\omega(\epsilon)}\right) (\epsilon \cos s + \epsilon^2 y_1(s) + \ldots) \, ds$$

$$= A\pi^2 \epsilon^3 + O(\epsilon^4).$$

Hence from equation (35),

$$\chi_1(0) = \frac{z_1(T(\epsilon))}{1 - \cos T(\epsilon)} = \frac{1}{2\pi A\epsilon} + O(\epsilon^0).$$

As $\epsilon \to 0^+$, equations (36) and (39) reproduce the $T \to 2\pi^+$ asymptotic behaviour observed in all the numerical experiments.

### 4.2 Vertical asymptotes

We have seen that a sign change in $\chi_1(0)$, and hence a transition from IPBs to APBs, must occur at $T = 2n\pi$ ($n \in \mathbb{Z}^+$) unless $z_1(2n\pi) = 0$, equation (36). In this section we will prove that, for a given $n$, the set of potentials on which (20) holds is negligibly small, so that the presence of asymptotes in the graphs of $\chi_1(0)$ against $T$ really is generic. To be precise, we will show that, for potentials in a certain Banach space $\mathcal{P}$, the subset of potentials on which (26) holds is locally a codimension 1 submanifold.
Definition 4 Let $P = \{ V : \mathbb{R} \to \mathbb{R} \text{ such that } V \text{ is } C^2 \text{ and } \| V \|_2 < \infty \}$ and $F : C^+_{T,T} \oplus P \to C^+_{T,0}$ 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 $V \in P$ is anharmonic at $q \in C^+_{T,2}$ if $q$ is nonconstant, $F(q, V) = 0$, and $\ker DF(q, V) = \{0\}$, where $DF(q, V) : C^+_{T,2} \to C^+_{T,0}$ 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 $(q, V) \in C^+_{T,2} \oplus P$ is a pair $(U, f)$ where $U \subset P$ is an open set containing $V$, and $f : U \to C^+_{T,2}$ is a $C^1$ map satisfying (a) every $W \in U$ is anharmonic at $f(W)$ and (b) $f(V) = q$. Note that $U$ is trivially a Banach manifold.

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

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 [3] for details). The open mapping theorem then ensures boundedness of $DF^{-1}(q, V)$. Hence $DF(q, V)$ is invertible, and the implicit function theorem applied to $F$ ensures existence of $(U, f)$ and local uniqueness of $f$. □

Definition 8 For $T \in 2\pi \mathbb{Z}^+$, we shall say that $V \in P$ 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 $T \in 2\pi \mathbb{Z}^+$, $V_0 \in P$ be degenerate at $q_0 \in C^+_{T,2}$, and $(U, f)$ be a perturbation neighbourhood of $(q_0, V_0)$. The subset of $U$ on which degeneracy persists is a codimension 1 submanifold.

Proof: Consider the $C^1$ mapping $I : U \to \mathbb{R}$ 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 $T_V U = P$ it splits and hence it suffices to show that $DI_V : P \to \mathbb{R}$ is surjective for all $V \in I^{-1}(0)$.

Let $V \in I^{-1}(0)$, $q = f(V)$. For any $\delta V \in P$, 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

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

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 $\delta V \in P$ such that $DI_V(\delta V) \neq 0$. We construct such a $\delta V$ 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 $\epsilon$ 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 $q^{-1} : [x_1, x_2] \to [t_0 - \epsilon, t_0 + \epsilon]$. 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 $C^1_K$ (the $C^1$ functions with support contained in $K$). Since $C^2_K$ is dense in $C^1_K$, there exists a sequence $\delta V_m \in C^2_K \subset P$ 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. □

In the above, we have chosen $P = (C^2(\mathbb{R}), \|\cdot\|_2)$ 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 $V_{G2}$) of the example potentials considered in section lie, strictly speaking, outside $P$, since they are unbounded. However, the analysis above can easily be adapted to deal with this: one simply replaces $P$ by the affine space $P_V := \{ W : \|W - V\|_2 < \infty \}$. 

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5 Concluding remarks

In this paper, breather initial profiles in the weak coupling regime of a simple class of oscillator networks have been examined, focusing on the dependence on breather period \( T \). The direction of continuation of one-site breathers was determined numerically using a simple and inexpensive numerical scheme. Two types of breather were identified, called IPBs and APBs. 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 [8]). Since APBs stress the central intersite springs more than IPBs they presumably make more effective seeds of mechanical breakdown.

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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 \( C \cap S = (0) \).

Note that if \( B \) is a Hilbert space then any closed subspace \( S \) splits since we can take the complement to be \( C = S^\perp \). Also if \( B \) is finite dimensional then since any subspace is closed all subspaces split. More generally 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 \( f : X \to Y \) between Banach manifolds is a submersion at \( x \in X \) if \( Df_x : T_x X \to T_{f(x)} Y \) 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 $T_xX$ 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 $f : X \to Y$ 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 $T_xf^{-1}(y) \cong \ker Df_x$.

The proof follows from working in charts around $x$ and $f(x)$ and applying the Implicit Function Theorem. For details of a proof see [1].

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