

Breathers in the weakly coupled topological discrete sine-Gordon system

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Abstract. Existence of breather (spatially localized, time periodic, oscillatory) solutions of the topological discrete sine-Gordon (TDSG) system, in the regime of weak coupling, is proved. The novelty of this result is that, unlike the systems previously considered in studies of discrete breathers, the TDSG system does not decouple into independent oscillator units in the weak coupling limit. The results of a systematic numerical study of these breathers are presented, including breather initial profiles and a portrait of their domain of existence in the frequency–coupling parameter space. It is found that the breathers are uniformly qualitatively different from those found in conventional spatially discrete systems.

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1. Introduction

Soliton dynamics in spatially discrete nonlinear systems plays a crucial part in the modelling of many phenomena in condensed matter and biophysics. One also encounters such systems in the numerical simulation of soliton dynamics in high energy physics where they arise as approximations of continuum models. In this case one is concerned with the extent to which these discretizations resemble their continuum counterparts—of course one hopes for a close resemblance. On the other hand, for applications in condensed matter and biophysics it is crucial that in certain respects the discrete systems have features not found in their continuum counterparts. One aspect in which recent work has revealed such a distinction is in the appearance of so-called breather solutions—that is spatially localized, time periodic solutions. Such solutions are conventionally called breathers, by analogy with the breathers of the continuum sine-Gordon equation. While it is rare for a nonlinear partial differential equation (PDE) to possess breather solutions (such solutions seem to be a feature of integrable systems), there has been mounting evidence that they are ubiquitous in spatially discrete systems. After numerical work and some heuristic arguments for the existence of such solutions, the existence of breathers in a weak coupling limit of a class of discrete systems was proved by MacKay and Aubry [1]. Subsequently these ideas were extended to a wider class of discrete systems by Sepulchre and MacKay [2]. The idea of both proofs is that each model has a parameter α , the coupling constant, and in the special case $\alpha = 0$ (called variously the anti-continuum, anti-integrable or weak coupling limit)

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the system decouples into independent oscillator units. If one sets one such unit oscillating while holding all others at rest, one obtains a trivial one-site (or unit) breather. Persistence of breathers in a sufficiently small neighbourhood of $\alpha = 0$ then follows from an implicit function theorem argument.

In this paper we present a study of breathers in the topological discrete sine-Gordon (TDSG) system [3]. The system is so called because it reduces to the sine-Gordon equation in the continuum limit, and because it preserves many of the ‘topological’ features of this equation, namely a topological lower bound on kink energy, and a continuous moduli space of static kinks saturating this bound. As a consequence of the preservation of these properties, kink dynamics in this system is remarkably close to that of its continuum counterpart, even in the highly discrete regime (kinks experience no Peierls–Nabarro barrier, and may propagate freely, indefinitely). One motivation for this work is to see whether this continuum-like behaviour extends to breathers also. The TDSG system falls just outside the scope of the existence theorems actually proved in [1, 2] (although both papers indicate that their methods *should* apply in situations not directly covered by the theorems they state). The reason is that there is no limit in which the system decouples into independent units. Nevertheless, the analysis of the model and, in particular, its kink solutions suggest that there is an anti-continuum-like limit. For example, there are one-site breathers in this limit and one suspects that despite the lack of complete decoupling the continuation methods of MacKay *et al* can be adapted to this setting. We show that this is indeed the case and prove a theorem about constant period continuation of the one-site breathers.

Furthermore, the continuation can be performed numerically by searching for fixed points of the period mapping of the system using a Newton–Raphson method, a technique developed for other systems by Aubry and Marín [4]. In this way we obtain a portrait of the period-coupling parameter space showing how far breathers of any particular period can be continued away from the zero coupling limit. We also obtain approximate breather initial profiles, and these display a rather unusual feature. Namely, the sites adjacent to the central oscillating site (the only one moving in the $\alpha = 0$ limit) shift away from equilibrium in the opposite direction to the central site. So the initial profiles are all, roughly speaking, sombrero shaped, rather than hump shaped as have usually been observed in discrete systems. The direction of continuation of breathers away from $\alpha = 0$ can be computed by a completely different (and very simple) numerical method, providing independent confirmation of this behaviour. The conclusion is, then, that breathers in the extremely discrete regime of the TDSG system are qualitatively quite different from those which appear in its continuum limit, and the two types of breather appear to be unrelated.

The rest of this paper is arranged as follows. Section 2 introduces the TDSG system and derives the one-site breathers in its weak coupling limit. In section 3, persistence of these breathers away from zero coupling, and exponential spatial localization of the continued breathers are proved. Section 4 presents the results of the numerical search for breathers using the Newton–Raphson method. In section 5 the direction of continuation is rederived by independent means. The work is summarized in section 6.

2. The topological discrete sine-Gordon system

The TDSG system (introduced by Ward and first studied in [3]) is a field theory in $1 + 1$ dimensions where space is discrete, with lattice spacing h , and time is continuous. It is most conveniently defined in the Lagrangian formalism. To each two-sided sequence $\psi : \mathbb{Z} \rightarrow \mathbb{R}$

one associates the potential energy

$$E_P[\psi] = \frac{h}{4} \sum_{n \in \mathbb{Z}} (D_n^2 + F_n^2) \quad (1)$$

where

$$D_n = \frac{2}{h} \sin \frac{1}{2}(\psi_{n+1} - \psi_n), \quad F_n = \sin \frac{1}{2}(\psi_{n+1} + \psi_n). \quad (2)$$

In the limit $h \rightarrow 0$, $D \rightarrow \psi_x$ and $F \rightarrow \sin \psi$, so E_P reduces to

$$E_P^{\text{cont}}[\psi] = \frac{1}{4} \int_{-\infty}^{\infty} (\psi_x^2 + \sin^2 \psi) dx, \quad (3)$$

the potential energy functional of the continuum sine-Gordon model. The key feature of this particular discretization is that

$$D_n F_n = -\frac{1}{h} (\cos \psi_{n+1} - \cos \psi_n), \quad (4)$$

so any configuration ψ satisfying kink boundary conditions

$$\lim_{n \rightarrow -\infty} \psi_n = 0, \quad \lim_{n \rightarrow \infty} \psi_n = \pi \quad (5)$$

is subject to the inequality

$$0 \leq \frac{h}{4} \sum_{n \in \mathbb{Z}} (D_n - F_n)^2 = E_P + \frac{1}{2} \sum_{n \in \mathbb{Z}} (\cos \psi_{n+1} - \cos \psi_n) = E_P - 1. \quad (6)$$

So $E_P \geq 1$ with equality if and only if $D_n = F_n$ for all n . Solutions of this first-order difference equation for ψ_n are minimizers of E_P among all sequences satisfying the kink boundary conditions (5), and hence static solutions of the model. The general solution of the first-order difference equation is

$$\psi_n = 2 \tan^{-1} e^{a(nh-b)} \quad (7)$$

where $a = h^{-1} \log[(2+h)/(2-h)]$ and b is a real-valued parameter, identified as the kink position. So, rather remarkably, the TDSG system has a continuous moduli space of static kinks (parametrized by $b \in \mathbb{R}$) and no Peierls–Nabarro barrier ($E_P = 1$ independent of b).

Dynamics is introduced into the system by defining the obvious kinetic energy

$$E_K = \frac{h}{4} \sum_{n \in \mathbb{Z}} \dot{\psi}_n^2. \quad (8)$$

The action functional is then $S[\psi] = \int (E_K - E_P) dt$. The Euler–Lagrange equations associated with this functional,

$$\ddot{\psi}_n = \frac{4-h^2}{4h^2} \cos \psi_n (\sin \psi_{n+1} + \sin \psi_{n-1}) - \frac{4+h^2}{4h^2} \sin \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1}) \quad (9)$$

provide the equations of motion for the TDSG. The analogue of the anti-continuum limit of this discrete system is not $h = \infty$, but rather $h = 2$, where the coefficient in front of the first term of (9) vanishes, and where the static kink solutions (7) degenerate to step-like functions. It is convenient to define a coupling constant

$$\alpha = \frac{4-h^2}{4h^2} \quad (10)$$

so that the ‘anti-continuum limit’ is $\alpha = 0$. In this limit the equations of motion reduce to

$$\ddot{\psi}_n = -\frac{1}{2} \sin \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1}). \quad (11)$$

Note that the lattice does not decouple into separate oscillators, but maintains nearest-neighbour interactions. Nevertheless, as was observed in [3] the $\alpha = 0$ system (11) has one-site breather solutions

$$\psi_n(t) = \begin{cases} 0 & n \neq 0 \\ \theta(t) & n = 0 \end{cases} \quad (12)$$

where $\theta(t)$ is any periodic solution of the pendulum equation

$$\ddot{\theta} + \sin \theta = 0. \quad (13)$$

We have chosen to locate the one-site breather at $n = 0$, but clearly any other site would do just as well. In fact, one could construct multisite breathers where any number of sites, none adjacent to any other, oscillate according to the pendulum equation, with periods in rational ratio. In this paper we will consider only one-site breathers, however.

As a system of autonomous differential equations, there is an \mathbb{R} -action on solutions of the TDSG system corresponding to the time translation symmetry of the system. Thus any breather solution gives rise to a one-parameter family of breathers. As a consequence, a breather solution is never an *isolated* solution [5]. To apply an implicit function theorem argument one needs to deal with this degeneracy—on the full phase space of the system the linearization of the equations of motion at a breather always has a non-trivial periodic solution which generates time translation along this breather. We deal with this by considering a subset of the phase space corresponding to solutions with a certain time reversal symmetry. We choose to work with solutions which are odd with respect to the time reversal symmetry, i.e. solutions that satisfy $\Psi(-t) = -\Psi(t)$ cf [1]. The main reason for this choice of symmetry is simply that odd solutions of the pendulum equation are simpler to write down in terms of elliptic functions than are even solutions. We will then prove that the continuation theorem in the space of odd functions implies a similar result in the space of even functions. Were we to consider continuation of multisite breathers, we would need to remove several phase degeneracies (one for each excited site) in order to apply the implicit function theorem. In fact the same procedure (restriction to odd solutions) removes all such degeneracies.

3. Continuation of one-site breathers: analytic results

Our proof of the existence of discrete breathers for the TDSG system in the weak coupling regime follows the method used by Aubry and MacKay in [1]. The proof proceeds in two steps; the first shows that certain periodic solutions persist and the second that these solutions continue to be exponentially localized. In this section, after introducing the function spaces we choose to work with, we state and prove the two halves of the continuation theorem.

3.1. The function spaces

Let $C_{T,2}^-$ denote the space of C^2 real-valued T -periodic functions on \mathbb{R} with odd time reversal symmetry. Equipped with the standard C^2 norm

$$|\psi|_2 = \sup_{t \in \mathbb{R}} \max \{ |\psi(t)|, |\dot{\psi}(t)|, |\ddot{\psi}(t)| \}, \quad (14)$$

$C_{T,2}^-$ becomes a Banach space. Similarly, let $C_{T,0}^-$ denote the space of C^0 real-valued T -periodic functions on \mathbb{R} with odd time reversal symmetry, equipped with the standard C^0 norm

$$|\psi|_0 = \sup_{t \in \mathbb{R}} \{ |\psi(t)| \}. \quad (15)$$

Consider the linear space $\oplus_{n \in \mathbb{Z}} X_n$, where each $X_n = C_{T,2}^-$, equipped with the natural sup norm, i.e. if $\Psi = (\psi_n)_{n \in \mathbb{Z}} \in \oplus_{n \in \mathbb{Z}} X_n$ then

$$\|\Psi\|_2 = \sup_{n \in \mathbb{Z}} |\Psi_n|_2. \quad (16)$$

Definition 1. $\Omega_{T,2}^- := \{\Psi \in \oplus_{n \in \mathbb{Z}} X_n : \|\Psi\|_2 < \infty\}$.

Similarly, equip the linear space $\oplus_{n \in \mathbb{Z}} Y_n$, where each $Y_n = C_{T,0}^-$, with its natural sup norm, i.e. if $\Psi = (\psi_n)_{n \in \mathbb{Z}} \in \oplus_{n \in \mathbb{Z}} Y_n$ then

$$\|\Psi\|_0 = \sup_{n \in \mathbb{Z}} |\Psi_n|_0. \quad (17)$$

Definition 2. $\Omega_{T,0}^- := \{\Psi \in \oplus_{n \in \mathbb{Z}} Y_n : \|\Psi\|_0 < \infty\}$.

Both $\Omega_{T,2}^-$ and $\Omega_{T,0}^-$ are Banach spaces. The equations of motion (9) give a natural map $F : \Omega_{T,2}^- \oplus \mathbb{R} \rightarrow \Omega_{T,0}^-$ defined by

$$F(\Psi, \alpha)_n = \ddot{\psi}_n - \alpha \cos \psi_n (\sin \psi_{n+1} + \sin \psi_{n-1}) + (\alpha + \frac{1}{2}) \sin \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1}). \quad (18)$$

The zeros of F correspond precisely to the odd T -periodic solutions of the equations of motion (9).

In section 2 we argued that $\alpha = 0$ should be considered as something akin to an anti-continuous limit for the TDSG system. Although the equations of motion (11) do not (in the terminology of MacKay and Sepulchre) decouple into *local units*, the energy density of the kink solutions becomes concentrated at one site—as one would demand for an anti-continuous limit. Moreover, like the models considered by Aubry and MacKay, at $\alpha = 0$ the system admits single site breather solutions—in our case the single non-stationary site moves according to the pendulum equation. So, analogously to the continuation of one-site breathers from the anti-continuous limit considered by various authors [1, 2, 4], one can ask what happens to these solutions as the coupling α is increased. Despite the somewhat different nature of the TDSG system we find similar continuation results to those of the authors mentioned above.

3.2. Statement of the continuation theorem

Given $T \in (2\pi, \infty) \setminus 2\pi\mathbb{N}$, denote by θ the unique odd T -periodic solution of the pendulum equation (13) with positive initial velocity. Let Θ denote the corresponding one-site breather solution of the TDSG at $\alpha = 0$ given by (12). Then we have the following theorem.

Theorem 3. *There exists $\epsilon > 0$ such that for $\alpha \in (0, \epsilon)$ there is a unique continuous family, Θ_α , of odd T -periodic solutions of TDSG at coupling α , such that $\Theta_0 = \Theta$. Moreover, these solutions are exponentially localized, i.e. there exist positive constants B and C (depending on T and α) such that $|(\Theta_\alpha)_n|_0 \leq C \exp(-B|n|)$ holds for all $n \in \mathbb{Z}$.*

In other words, for small enough α the one-site breather Θ has a locally unique continuation among odd T -periodic solutions and these continued solutions remain exponentially localized. The proof of this theorem is given in the next two sections. Section 3.3 establishes the continuation through T -periodic solutions while section 3.4 deals with the question of localization.

3.3. Persistence of periodicity

By our remark in section 3.1, Ψ is an odd solution of the TDSG system with period T for coupling α , if and only if, $F(\Psi, \alpha) = \mathbf{0}$ for the function F defined by equations (18). The odd one-site breather Θ of period T gives us a solution for $\alpha = 0$. The proof proceeds by showing that F is a C^1 function to which the implicit function theorem may be applied. Thus a locally unique zero (and hence an odd T -periodic solution of TDSG) of F for α close enough to 0 is demonstrated. It remains to show that the implicit function theorem can be applied to F , i.e. we need to check that F is C^1 and that DF , its derivative with respect to the $\Omega_{T,2}^-$ factor is invertible at the one-site breather solution.

Proof. The verification of the first fact is straightforward. A short computation gives us the following. If we let

$$DF : (\Omega_{T,2}^- \oplus \mathbb{R}) \oplus (\Omega_{T,2}^- \oplus \mathbb{R}) \longrightarrow \Omega_{T,0}^- \quad (19)$$

be the derivative of F and write

$$DF_{\Psi,\alpha}(\delta\Psi, \delta\alpha) = (\tilde{\psi}_n)_{n \in \mathbb{Z}} \quad (20)$$

then DF is defined by

$$\begin{aligned} \tilde{\psi}_n = & \delta\ddot{\psi}_n - [\sin \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1}) - \cos \psi_n (\sin \psi_{n+1} + \sin \psi_{n-1})] \delta\alpha \\ & + [\alpha \sin \psi_n (\sin \psi_{n+1} + \sin \psi_{n-1}) + \beta \cos \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1})] \delta\psi_n \\ & - \alpha \cos \psi_n (\cos \psi_{n+1} \delta\psi_{n+1} + \cos \psi_{n-1} \delta\psi_{n-1}) \\ & + \beta \sin \psi_n (\sin \psi_{n+1} \delta\psi_{n+1} + \sin \psi_{n-1} \delta\psi_{n-1}), \end{aligned} \quad (21)$$

where $\beta = \alpha + \frac{1}{2}$. From this it is easily seen that DF is bounded. At $\alpha = 0$, DF , the derivative of F with respect to the $\Omega_{T,2}^-$ factor, reduces to

$$\begin{aligned} DF_{\Psi}(\delta\Psi)_n = & \delta\ddot{\psi}_n + \frac{1}{2} \cos \psi_n (\cos \psi_{n+1} + \cos \psi_{n-1}) \delta\psi_n \\ & + \frac{1}{2} \sin \psi_n (\sin \psi_{n+1} \delta\psi_{n+1} + \sin \psi_{n-1} \delta\psi_{n-1}). \end{aligned} \quad (22)$$

In general this is a tridiagonal but not diagonal operator. However, DF evaluated at any one-site breather is diagonal. Explicitly, substituting $\Psi = \Theta$, the one-site breather of the form (12), into (22) yields $DF_{\Theta} = \oplus_{n \in \mathbb{Z}} L_n$, where $L_n : C_{T,2}^- \rightarrow C_{T,0}^-$ is,

$$L_n(\psi) = \begin{cases} \ddot{\psi} + \cos \theta \psi & \text{if } n = 0, \\ \ddot{\psi} + \frac{1}{2}(1 + \cos \theta) \psi & \text{if } n = \pm 1, \\ \ddot{\psi} + \psi & \text{otherwise.} \end{cases} \quad (23)$$

Clearly, to prove invertibility of DF at a one-site breather it is sufficient to prove that each operator L_n is invertible, since then $DF^{-1} = \oplus_{n \in \mathbb{Z}} L_n^{-1}$ and we see that $\|DF^{-1}\| \leq \max\{|L_0^{-1}|, |L_1^{-1}|, |L_2^{-1}|\}$. Invertibility of the operator L_n will follow (see section 3.3.2) from standard facts about linear differential equations once we establish that $\ker L_n = \{0\}$.

3.3.1. Injectivity of DF_{Θ} . For $T \notin 2\pi\mathbb{Z}$, one sees immediately that $\ker L_n = \{0\}$ for $|n| > 1$. So it remains to consider the central ($n = 0$) and off-central ($n = \pm 1$) equations

$$\ddot{\psi} + \cos \theta \psi = 0 \quad (24)$$

$$\ddot{\psi} + \frac{1}{2}(1 + \cos \theta) \psi = 0 \quad (25)$$

where θ is a T -periodic, odd solution of the pendulum equation, $\ddot{\theta} = -\sin\theta$, with positive initial velocity. Both (24) and (25) are Hill equations, that is ordinary differential equations (ODEs) of the form $\ddot{\psi} = q(t)\psi$ where q is periodic. Such equations have a long history. They arise, for example, in stability analyses of celestial mechanics [6]. Note that in both (24) and (25) the potential, $q(t)$, has basic (i.e. smallest) period $T/2$ since \cos is even. Such equations may have periodic solutions only with basic period not less than $T/2$. To prove that L_0 and $L_{\pm 1}$ have trivial kernel, we will have to prove separately the non-existence of $T/2$ - and T -periodic odd solutions of (24) and (25).

This task is simplified slightly for equation (24) by the observation that $\psi = \dot{\theta}$ is an even T -periodic solution. This is, in fact, a consequence of the time translation symmetry of one-site breather solutions previously mentioned. A standard result of Floquet theory [7] implies that (24) cannot have both $T/2$ -periodic and T -periodic solutions, so it suffices in this case to rule out existence of T -periodic odd solutions. No such simplification occurs for the off-central equation (25).

To proceed further one must consider the specific form of the solution θ of the pendulum equation. If $\theta(0) = 0$ and $\dot{\theta}(0) = 2k$, where $k \in (0, 1)$ then the solution has amplitude of oscillation $\theta_0 \in (0, \pi)$ satisfying $\theta_0 = 2 \arcsin k$, and period $T = 4K$ where

$$K = \int_0^{\frac{\pi}{2}} \frac{dz}{\sqrt{1 - k^2 \sin^2 z}} \quad (26)$$

is the complete elliptic integral of the first kind [8]. The parameter k is called the modulus in the literature on elliptic functions. In fact this solution satisfies

$$\sin \frac{1}{2}\theta(t) = k \operatorname{sn} t \quad (27)$$

where sn is the sn-oidal elliptic function of Jacobi. Note that sn itself, like all elliptic functions, depends parametrically on k . This dependence will always be suppressed in our notation. Substitution of (27) into (24), (25) recasts them as a pair of Lamé equations [9],

$$\ddot{\psi} + (1 - 2k^2 \operatorname{sn}^2 t)\psi = 0 \quad (28)$$

$$\ddot{\psi} + (1 - k^2 \operatorname{sn}^2 t)\psi = 0. \quad (29)$$

A standard technique when seeking $2K$ - and $4K$ -periodic solutions of a Lamé equation is to make the following elliptic change of time coordinate,

$$t \mapsto x(t) = \operatorname{am}(t) \quad (30)$$

where am is Jacobi's amplitude function, that is, the unique continuous function satisfying $\sin x(t) = \operatorname{sn} t$, $x(0) = 0$. Under this coordinate change the pair of Lamé equations above becomes a pair of Ince equations [9],

$$(1 + a \cos 2x)\psi'' - a \sin 2x \psi' + (1 - a + 2a \cos 2x)\psi = 0 \quad (31)$$

$$(1 + a \cos 2x)\psi'' - a \sin 2x \psi' + (1 + a \cos 2x)\psi = 0 \quad (32)$$

where ψ' denotes $d\psi/dx$ etc, and $a = k^2/(2 - k^2)$ is a period-dependent parameter taking values in $(0, 1)$. Note that the coefficients in these ODEs are periodic in x with period π , independent of k , and hence T . So all k dependence is now explicit and resides in the constant $a(k)$. Odd $2K$ - and $4K$ -periodic solutions of (28), (29) correspond to odd π - and 2π -periodic solutions of (31), (32), and vice versa.

So, we need to prove that (31) has no odd 2π -periodic solutions, and that (32) has neither 2π - nor π -periodic odd solutions. Assume, to the contrary, that such solutions exist. Let ψ^1, ψ^2 be 2π -periodic odd solutions of (31) and (32) respectively, and ψ^3 be a

π -periodic odd solution of (32). Functions of such parity and periodicity must have purely sinusoidal Fourier expansions of the following forms:

$$\begin{aligned}\psi^\sigma &= \sum_{n=1}^{\infty} A_n^\sigma \sin(2n-1)x & \sigma = 1, 2 \\ \psi^3 &= \sum_{n=1}^{\infty} A_n^3 \sin 2nx.\end{aligned}\tag{33}$$

Since the coefficients in (31) and (32) are analytic in x , each $\psi^\sigma(x)$ is analytic in a strip of the complex x plane containing the real axis [10]. It follows that the Fourier coefficients A_n^σ , $\sigma = 1, 2, 3$, must satisfy strong decay criteria, namely

$$\lim_{n \rightarrow \infty} n^p A_n^\sigma = 0\tag{34}$$

for every $p \geq 0$. Substituting the Fourier expansions for ψ^σ into their appropriate Ince equations one obtains the following linear second-order difference equations for A_n^σ :

$$\begin{aligned}A_1^1 + A_2^1 &= 0, \\ A_{n+1}^1 + \frac{4n^2 - 4n + a}{a(2n-1)(n+1)} A_n^1 + \frac{n-2}{n-1} A_{n-1}^1 &= 0 \quad n \geq 2;\end{aligned}\tag{35}$$

$$\begin{aligned}A_1^2 + 5A_2^2 &= 0, \\ A_{n+1}^2 + \frac{8n(n-1)}{a(4n^2 + 2n - 1)} A_n^2 + \frac{4n^2 - 10n + 5}{4n^2 + 2n - 1} A_{n-1}^2 &= 0 \quad n \geq 2;\end{aligned}\tag{36}$$

$$\begin{aligned}6A_1^3 + 11aA_2^3 &= 0, \\ A_{n+1}^3 + \frac{2(4n^2 - 1)}{a(4n^2 + 6n + 1)} A_n^3 + \frac{4n^2 - 6n + 1}{4n^2 + 6n + 1} A_{n-1}^3 &= 0 \quad n \geq 2.\end{aligned}\tag{37}$$

Lemma 4. For all $a \in (0, 1)$, all non-trivial solutions of the difference equations (35)–(37) are exponentially divergent. (By trivial we mean identically zero.)

The proof of this lemma is straightforward, but rather involved. The interested reader is directed to the appendix.

Since none of the sequences A_n^σ satisfy the decay criterion (34), we conclude that no such solutions ψ^σ exist. Hence $\ker L_0 = \ker L_{\pm 1} = \{0\}$.

3.3.2. Invertibility. Having established that each L_n as a linear operator $C_{T,2}^- \rightarrow C_{T,0}^-$ is injective, we apply standard linear ODE theory to show that each L_n is invertible (i.e. its inverse is bounded). Consider L_n acting on the full space $C_{T,2} \rightarrow C_{T,0}$. Each L_n respects the splittings $C_{T,*} = C_{T,*}^+ \oplus C_{T,*}^-$, where $C_{T,*}^+$ denotes the subspace of even loops.

Lemma 5. $\ker L_n \subset C_{T,2}^+$.

Proof. This is immediate from previous work except for the cases $|n| = 1$. Suppose $\psi = \psi^+ + \psi^- \in C_{T,2}$ and $L_n \psi = 0$. Then since L_n preserves the odd–even splitting, we must have $L_n \psi^+ = L_n \psi^- = 0$ and hence $\psi^- = 0$, by the previous section. \square

Let $\ker L_n^\perp = \{\psi \in C_{T,0} : \langle \psi, \ker L_n \rangle_2 = 0\}$, where $\langle \cdot, \cdot \rangle_2$ is the standard L^2 inner product.

Corollary 6. $C_{T,0}^- \subset \ker L_n^\perp$.

Proposition 7. Each $L_n : C_{T,2}^- \rightarrow C_{T,0}^-$ is an invertible linear map.

Proof. Standard linear ODE theory implies that $L_n : C_{T,2} \rightarrow \ker L_n^\perp$ is surjective. In particular, $L_n : C_{T,2} \rightarrow C_{T,0}^- \subset \ker L_n^\perp$ is surjective. But since L_n preserves the odd–even splitting, $L_n : C_{T,2}^- \rightarrow C_{T,0}^-$ is still surjective. Now we have a bounded, injective, surjective linear map and hence the closed graph theorem implies that L_n has a bounded inverse. \square

3.4. Exponential localization

We now turn to the question of localization. Issues related to exponential localization in the general class of *networks* have been treated by MacKay and Baesens in [11]. Localization of our continued periodic solutions will follow from an application of their results. To state the relevant results from [11] we need to recall some definitions from that paper.

Consider a *network*, that is a countable metric space S with metric d (in our case $S = \mathbb{Z}$ with $d(m, n) = |m - n|$). To each $s \in S$ associate two normed spaces X_s and Y_s , with norms $|\cdot|_{X_s}$ and $|\cdot|_{Y_s}$, to be considered as a local state space and a local force space respectively—in our case each X_s is the space of C^2 odd T -periodic loops in \mathbb{R} with the norm given by equation (14) and each Y_s is the space of C^0 odd T -periodic loops in \mathbb{R} with the norm given by equation (17). Define X by

$$X = \left\{ x \in \bigoplus_s X_s : \|x\|_X := \sup_{s \in S} |x_s|_{X_s} < \infty \right\} \tag{38}$$

and Y similarly (in our case $X = \Omega_{T,2}^-$, $Y = \Omega_{T,0}^-$ and the norms on X and Y are just those already given on these spaces of loops in section 3).

Definition 8. A bounded linear map $L : X \rightarrow Y$ is said to be ϕ -exponentially local if there exists $\epsilon > 0$ and a continuous function $\phi : [0, \epsilon) \rightarrow \mathbb{R}$ such that

$$\sup_{r \in S} \sum_{s \in S} |L_{rs}| z^{d(r,s)} \leq \phi(z), \quad z \in [0, \epsilon). \tag{39}$$

The tridiagonal linear map $DF_\Theta : \Omega_{T,2}^- \rightarrow \Omega_{T,0}^-$ is an exponentially local map (e.g. we can take $\phi(z) = \|DF_\Theta\|(2z + 1)$).

Definition 9. $u \in Y$ (or in X) is (C, λ) -exponentially localized about a site $o \in S$, if there exist $C > 0$, $0 < \lambda < 1$ such that $|u_s| \leq C\lambda^{d(s,o)}$.

Certainly, a one-site breather is exponentially localized about the single oscillating site o (e.g. we can take $C = |u_o|$, and any $\lambda > 0$). We now state the main result of [11].

Theorem 10 (Baesens–MacKay). *If $L : X \rightarrow Y$ is ϕ -exponentially local and invertible, and $u \in Y$ is (C, λ) -exponentially localized about site $o \in S$, then $L^{-1}u$ is (WC, μ) -exponentially localized about o , where W and μ depend only on $\|L^{-1}\|$, λ and a function β related to the function ϕ .*

As an application of the above theorem, MacKay and Baesens prove a theorem concerning continuation problems. Let $F : \mathbb{R} \oplus X \rightarrow Y$ be a C^1 function, which at $\alpha = 0$ has a regular zero, i.e. there is a solution Θ_0 of $F(0, \Theta) = 0$ at which DF_0 is invertible. Then, by the implicit function theorem there is a neighbourhood of 0 in which $F(\alpha, \Theta) = 0$ has a unique solution Θ_α close to Θ_0 . The solution satisfies

$$\frac{d\Theta_\alpha}{d\alpha} = -L_\alpha^{-1} \left(\frac{dF}{d\alpha}(\Theta_\alpha, \alpha) \right) \tag{40}$$

where $L_\alpha = DF_\alpha(\Theta_\alpha)$ and may be continued as long as L_α remains invertible. In this setting they prove the following theorem.

Theorem 11 (Baesens–MacKay). *Suppose Θ_0 is exponentially localized about site $o \in S$, with continuation Θ_α for $\alpha \in [0, \alpha_0]$ and with L_α ϕ -exponentially local. If $\frac{dF}{d\alpha}(\Theta_0)$ is (A, μ) -exponentially localized about o , $F \in C^2$, and $\frac{d}{d\alpha}DF$ is ψ -exponentially local for $|\Theta| \leq \sup_{\alpha \in [0, \alpha_0]} |\Theta_\alpha|$ and $\alpha \in [0, \alpha_0]$, then Θ_α is exponentially localized about o for $\alpha \in [0, \alpha_0]$.*

We have shown that for the function F defined by (18), for each $T \in (2\pi, \infty) \setminus 2\pi\mathbb{N}$ the odd one-site breather, Θ_0 of period T is a regular zero of F . Choose $\alpha_0 > 0$ so that for $\alpha \in [0, \alpha_0]$ the continuation Θ_α exists. We claim that the conditions of theorem 11 obtain. For each $\alpha \in [0, \alpha_0]$, L_α is ϕ -exponentially local where $\phi(z) = A(2z + 1)$ and $A = \max_{\alpha \in [0, \alpha_0]} \|L_\alpha\|$. From

$$\frac{dF}{d\alpha}(\Theta_0)_n = \begin{cases} 2 \sin \theta & \text{if } n = 0, \\ -\sin \theta & \text{if } |n| = 1, \\ 0 & \text{otherwise} \end{cases} \quad (41)$$

we see that $\frac{dF}{d\alpha}(\Theta_0)$ is exponentially localized about $n = 0$. It follows from

$$\begin{aligned} \frac{d}{d\alpha}DF_\Psi(\delta\Psi)_n &= [(\cos(\psi_{n+1} - \psi_n) + \cos(\psi_{n-1} - \psi_n))\delta\psi_n \\ &\quad + \cos(\psi_{n+1} + \psi_n)\delta\psi_{n+1} + \cos(\psi_{n-1} + \psi_n)\delta\psi_{n-1}] \end{aligned} \quad (42)$$

that $\frac{d}{d\alpha}DF$ is ψ -exponentially local for $\psi(z) = 2(1 + z)$. It is straightforward to check that F is C^2 . Hence theorem 11 may be applied in our situation: the continued periodic solutions Θ_α remain exponentially localized and thus are discrete breathers as claimed. \square

3.5. Continuation of even breathers

We have proved that for any $T \in (2\pi, \infty) \setminus 2\pi\mathbb{N}$ there exists a locally unique continuation Θ_α through $\Omega_{T,2}^-$ of the odd one-site breather Θ . The purpose of this section is to prove that a similar result holds for continuation of *even* one-site breathers also. Since this is not quite so obvious as it may seem, we will state and prove this result carefully. Let $\Omega_{T,n}$ be the space of all T -periodic C^n loops, and $\Omega_{T,n}^+$ be its even subspace, both equipped with their natural norms (see section 3.1). Translating Θ , the odd one-site breather of period T , through a time of $T/4$ one clearly obtains an even one-site breather, call it $\tilde{\Theta}$ (so explicitly, $\tilde{\Theta}(t) = \Theta(t + T/4)$). Note this is a slight abuse of notation: we are using Θ to represent both a point in $\Omega_{T,2}^-$ and the value of the corresponding function at a particular time). If one similarly translates the family Θ_α , one obtains a continuation $\tilde{\Theta}_\alpha$ of $\tilde{\Theta}$ through breather solutions in $\Omega_{T,2}$. We will prove that, for α small enough, this continuation actually lies in the even subspace $\Omega_{T,2}^+$.

Corollary 12. *For each $T \in (2\pi, \infty) \setminus 2\pi\mathbb{N}$ there exists $\epsilon > 0$ such that there is a locally unique continuous family $\tilde{\Theta}_\alpha \in \Omega_{T,2}^+$ of solutions of the TDSG system at coupling $\alpha \in [0, \epsilon)$, with $\tilde{\Theta}_0 = \tilde{\Theta}$. These solutions are exponentially localized.*

Proof. By theorem 3 there exists $\epsilon > 0$ such that for $\alpha \in [0, \epsilon)$ there is a continuous family $\Theta_\alpha \in \Omega_{T,2}^-$ of odd breather solutions with $\Theta_0 = \Theta$. Choosing ϵ sufficiently small, each Θ_α is unique (i.e. is the only zero of F) in the open ball $B_\epsilon(\Theta) \subset \Omega_{T,2}^-$. Consider the family

$\tilde{\Theta}_\alpha$ defined by $\tilde{\Theta}_\alpha(t) = \Theta_\alpha(t + T/4)$. Clearly $\tilde{\Theta}_\alpha$ is a continuation of the even one-site breather $\tilde{\Theta}$ through exponentially localized breathers in $\Omega_{T,2}$. It remains to prove that this continuation actually lies in $\Omega_{T,2}^+$.

For each $\alpha \in (0, \epsilon)$ define another breather solution $\hat{\Theta}_\alpha$ of the TDSG system by $\hat{\Theta}_\alpha(t) = -\Theta_\alpha(t + T/2)$. By periodicity and oddness of Θ_α one sees that $\hat{\Theta}_\alpha \in \Omega_{T,2}^-$. Also, $\|\hat{\Theta}_\alpha - \Theta\|_2 \equiv \|\Theta_\alpha - \Theta\|_2 < \epsilon$ since the one-site breather Θ satisfies the identity $\Theta(t + T/2) \equiv -\Theta(t)$. But the continuation Θ_α is unique in the ball $B_\epsilon(\Theta) \subset \Omega_{T,2}^-$, so we conclude that $\hat{\Theta}_\alpha = \Theta_\alpha$. Hence $\hat{\Theta}_\alpha(T/2) = -\hat{\Theta}_\alpha(0)$, and by time reversal symmetry of the TDSG system, $\hat{\Theta}_\alpha(T/4) = \mathbf{0}$. But $\hat{\Theta}_\alpha(0) = \hat{\Theta}_\alpha(T/4) = \mathbf{0}$, so $\tilde{\Theta}_\alpha$ is even.

Local uniqueness of the even continuation $\tilde{\Theta}_\alpha$ is immediate. For if the continuation were not unique on a small enough neighbourhood of Θ , one would be able to construct an alternative odd continuation, again by time translation, in violation of local uniqueness of Θ_α . \square

4. Continuation of one-site breathers: numerical results

For each non-resonant period T , corollary 12 yields a one-parameter family of T -periodic even breathers, but fails to give detailed information about these solutions. For example, it gives little information about the domain of existence of the continuation, how this domain varies with the period T , or the profiles of the breathers. We have obtained some such information through numerical work. This section describes in detail the numerical scheme used and the results obtained.

Before describing the numerical work we note that there is one established mechanism which puts limits on the extent of the continuation being attempted. Namely, one expects unique continuation to fail once the breather enters into resonance with the phonons of the system. Linearizing the equations of motion about the vacuum and seeking solutions of travelling wave type yields the phonon dispersion relation

$$\omega^2 = 1 + 4\alpha \sin^2 \frac{k}{2} \quad (43)$$

relating frequency ω to wavenumber k [3]. From this we see that the phonon frequency band at coupling α is $[1, \sqrt{1 + 4\alpha}]$. Suppose we fix a frequency $\omega \in (n^{-1}, (n-1)^{-1})$, $n = 2, 3, \dots$ so that its lowest harmonic above the bottom edge of the phonon band is $n\omega$. Then during continuation of the frequency ω one-site breather, α increases from 0 and the phonon band expands, eventually capturing the harmonic $n\omega$ when $n\omega = \sqrt{1 + 4\alpha}$ (if continuation persists this far). Beyond this point one expects not only loss of uniqueness of the continuation, but also a breakdown in exponential localization [12], since the phonons themselves are not localized. Thus the union of the curves

$$\alpha = \frac{1}{4}(n^2\omega^2 - 1), \quad n^{-1} < \omega < (n-1)^{-1}, \quad n = 2, 3, \dots \quad (44)$$

with vertical line segments at the resonant frequencies $\omega = n^{-1}$ provides an upper boundary to the possible breather existence domain in the (ω, α) parameter space (see figure 1). We will find that the existence domain is considerably smaller than the region bounded by this curve.

The idea behind the numerical method used to map out the existence domain is to convert the existence proof of section 3 into a constructive means of finding periodic solutions. By the analysis of that section, we know that the nonlinear function F defined therein is invertible at a one-site breather (provided the frequency of the breather is non-resonant) and

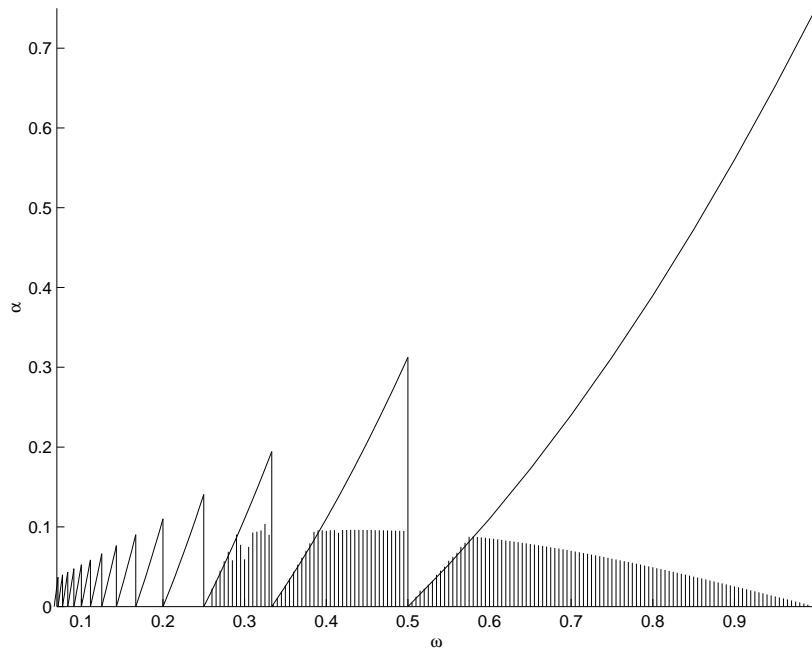


Figure 1. The continuation domain of one-site breathers in (ω, α) space. The upper, jagged curve is the boundary obtained from the phonon resonance argument, and consists of parabolic segments. The shaded region beneath this curve is the actual continuation domain obtained by numerical analysis for $\omega \in [0.25, 1]$, one vertical line for each frequency sampled. The region to the left of $\omega = 0.25$ is inaccessible to our numerical scheme.

hence, by the implicit function theorem, we know that in a neighbourhood of the one-site breather, $F^{-1}(0)$ is a smooth curve. This curve is the one-parameter family of periodic solutions we seek, parametrized by the coupling α . Given one point on the curve (e.g. the one-site breather at $\alpha = 0$) one can find sufficiently close neighbouring points by using the given point as initial input in a root-finding algorithm for F . Working piecemeal from $\alpha = 0$, we can in this way construct the entire curve. To solve $F = 0$ we may use a Newton–Raphson method, which will converge provided DF is invertible at the root and we attempt a small enough step along the curve.

As it stands, this scheme is impractical since the spaces on which F is defined are infinite dimensional. We may seek a finite-dimensional truncation of the scheme in several ways. One approach is to truncate the lattice to finite size, and approximate the space of periodic functions associated with each lattice site by some finite Fourier series representation. Then the problem is reduced to that of determining the finite number of Fourier coefficients at the finite number of lattice sites, which is solvable by Newton–Raphson. This is somewhat complicated in the TDSG system because one must compute Fourier transforms of non-polynomial nonlinear terms, necessitating the use of fast Fourier transforms [13].

For this reason we prefer an alternative approach, where F is replaced by a function stemming from the Poincaré return map for period T , which we shall denote T . We again truncate the lattice to finite size (say $2N+1$ sites symmetrically distributed about the breather centre), and consider the map on phase space which maps the initial data of a solution to its phase space position after time T . This map may be computed in practice by solving the lattice equations of motion using a fourth-order Runge–Kutta method. Fixed points

of the map T , or equivalently, zeros of $T - \text{Id}$, are clearly periodic solutions. However, on the whole phase space, solutions are never isolated because of the time translation symmetry. Consequently, DT is never invertible, and hence we cannot directly apply a Newton–Raphson algorithm.

The solution to this difficulty is to consider some restriction of T which has no such time-translation symmetry. Marín and Aubry [4] consider the restricted return map $T_P : \mathbb{R}^{2N+1} \rightarrow \mathbb{R}^{2N+1}$ which takes initial positions of time reversal symmetric solutions (so that initial velocity is 0) to their positions at time T . That fixed points of T_P are truly T -periodic is an immediate consequence of energy conservation. An unfortunate consequence of this choice is that at $\alpha = 0$, $D(T_P - \text{Id})$ is singular for all ω . Explicitly,

$$DT_P = \text{diag}(\cos T, \dots, \cos T, y_1(T), y_0(T), y_1(T), \cos T, \dots, \cos T), \quad (45)$$

where y_0, y_1 are solutions of (24), (25) respectively with initial data $y_n(0) = 1, \dot{y}_n(0) = 0, \theta$ now being the *even* T -periodic solution of the pendulum equation. Let \bar{y}_0 be the odd solution of (24) with $\bar{y}_0(0) = 1$. Then a short calculation reveals that $\bar{y}_0(t) = -\theta(t)/\sin\theta(0)$ which is T -periodic. Conservation of the Wronskian $y_0\dot{\bar{y}}_0 - \dot{y}_0\bar{y}_0$ then implies that $y_0(T) = 1$. Hence $\det(DT_P - \mathbb{I}) = 0$, and one is not guaranteed good behaviour of the Newton–Raphson algorithm for $T_P - \text{Id}$ at, and close to, $\alpha = 0$. This problem is not specific to the TDSG system, and was in fact pointed out in [4].

An alternative restriction, which we denote T_V , arises by mapping the initial position of a time reversal symmetric solution to its velocity after one period. Certainly, T -periodic solutions are zeros of T_V , although the converse is clearly false since the $2T$ -periodic one-site breather is a zero of T_V at $\alpha = 0$. (In fact any zero of T_V *must* be $2T$ -periodic by time reversal symmetry of the system.) This is not a problem provided the zero we seek is isolated, which is guaranteed by the inverse function theorem so long as DT_V remains invertible along the continuation curve. The advantage of this approach is that at $\alpha = 0$,

$$DT_V = \text{diag}(-\sin T, \dots, -\sin T, \dot{y}_1(T), \dot{y}_0(T), \dot{y}_1(T), -\sin T, \dots, -\sin T), \quad (46)$$

which turns out to be non-singular except at the resonant periods $T = 2n\pi$, where continuation is not expected anyway, and also at the ‘false resonances’ $T = (2n + 1)\pi$. As continuation proceeds, care must be taken, once a zero of $\det DT_V$ has been encountered, that we do not follow a spurious, non-periodic branch of $T_V^{-1}(0)$. At the end of the Newton–Raphson algorithm we check separately that the proposed periodic solution really is a fixed point of T_P to within numerical tolerance (note that this involves no extra computational cost since T_P is an inevitable by-product of the calculation of T_V). So it is possible that the continuation could fail prematurely at a zero of DT_V if it is diverted from the true curve onto a spurious branch. This turns out to be a problem only around the false resonant frequency $\omega = \frac{2}{7}$ in our work (see discussion below).

To test whether the continuation has failed we use two criteria, beyond mere failure of the Newton–Raphson algorithm to converge. First, we check that each new solution does not differ greatly from the previous one, by computing $\|\Theta_{\alpha_1} - \Theta_{\alpha_0}\|_2$. This is to ensure that the continuation has not jumped across to some distant zero of T_V , as Newton–Raphson output is wont to do close to singular points. Second, we seek bifurcations of the continuation by applying a simple, necessary, but not sufficient, test. Namely, we terminate continuation if ever $\det DT_V$ and $\det DT_P$ *simultaneously* vanish (note that this test requires minimal extra computational effort since DT_V is required by the Newton–Raphson algorithm, and cannot be calculated without producing DT_P as a by-product. The only extra cost is that of the *LU* decomposition of DT_P , insignificant compared with the cost of the Runge–Kutta method). That this test is not sufficient is clear from

consideration of the false resonant frequencies $\omega = \frac{2}{n}$ at $\alpha = 0$, where no bifurcation can exist by corollary 12. A full bifurcation analysis, along the lines of [13], would remedy this insufficiency, but only at considerable computational cost, and would be well beyond the scope of this paper. We hope to perform such an analysis in the future.

The results of the continuation algorithm, using a 13-site lattice with fixed endpoints and the implementations of the Runge–Kutta and Newton–Raphson methods outlined in [14], are presented in figure 1. The phonon resonance boundary clearly curtails continuation just to the right of the resonant frequencies $\omega = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$. However, for large regions of ω space, continuation fails before phonon resonance can occur, at what appear to be genuine bifurcations (at least $\det DT_V = \det DT_P = 0$) the underlying physical mechanism for which remains mysterious. The exception is a small ω range around the false resonance $\omega = \frac{2}{7}$ where the continuation seems to fail spuriously due to its encountering a zero of $\det DT_V$ which is not a genuine bifurcation point ($\det DT_P \neq 0$), but which derails the Newton–Raphson algorithm nonetheless. The $\omega \in [0.27, 0.3]$ part of figure 1 should thus be viewed with a little scepticism.

Closer examination of the results around $\omega = \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$ (figure 2) reveals that the continuation slightly oversteps the resonance boundary defined by equation (44). This can be well understood as a finite size effect: equation (43) is the dispersion relation for an infinite lattice, whereas we have a $2N + 1$ site lattice, divided by the central site into two ‘tails’ of length N which remain close to the vacuum. The relevant spectrum for small amplitude oscillations is doubly degenerate, consisting of two copies of the normal mode spectrum of the N -site linearized lattice (one copy for each of the two tails), which itself consists of N distinct frequencies ω_j , $j = 1, 2, \dots, N$, easily shown [15] to satisfy

$$\omega_j^2 = 1 + 4\alpha \sin^2 \left(\frac{j\pi}{2N+2} \right). \quad (47)$$

So bifurcation should be expected at that value of α for which ω_N coincides with the lowest harmonic of ω above 1. This leads to a slightly different boundary from that previously discussed. Since the ‘phonon’ spectrum is now discrete, it is possible for the continuation to skip over this first bifurcation point occasionally, and detect a later one instead, due to ω_{N-1} , ω_{N-2} etc. In our case, $N = 6$, so there are six parabolic resonance curves, one for each normal mode frequency. These are included in figure 2.

As a by-product of the numerical work described above we also obtain breather initial profiles within the continuation domain. The resulting profiles are highly spatially localized, and remarkably uniform, all exhibiting basically the same shape: compared with the one-site breather of the same period, the central site of the continued breathers is displaced slightly more than in the one-site breather, the two adjacent sites are displaced negatively by a small amount, and the remaining sites are barely displaced at all. Figure 3 shows breather profiles of the same frequency at increasing coupling, and profiles at the same coupling and various frequencies. Breather shape will be discussed further in the next section.

Finally, we remark that the numerical methods described above are inefficient for investigating the long-period breathers of the system. Indeed, if one used the same time step in the numerical integration schemes independent of the period, T , then of course the time to compute T_V and DT_V , which occupies the vast majority of the computing time, would grow linearly with T . If one wanted to investigate long-period breathers then it would seem more efficient to switch from the Runge–Kutta scheme to a symplectic integrator, of which one expects reliable long-time integration at modest time step size. The efficiency of the algorithm could also be improved by enabling it to take larger steps in α so that the

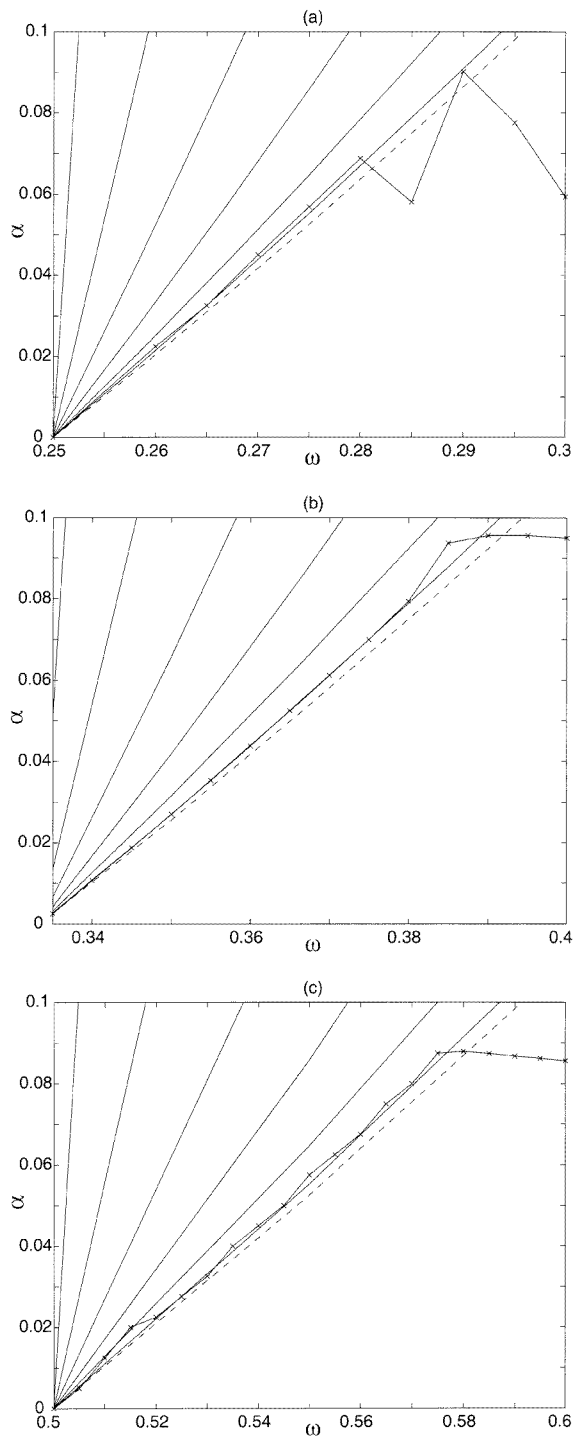


Figure 2. Details of the continuation domain around three resonant frequencies: (a) $\omega = \frac{1}{4}$, (b) $\omega = \frac{1}{3}$ and (c) $\omega = \frac{1}{2}$. In each case, the full curve with crosses represents the numerical results, the broken curve is the phonon resonance boundary for an infinite lattice, and the six full curves without crosses are the parabolic resonance curves for the 13-site lattice.

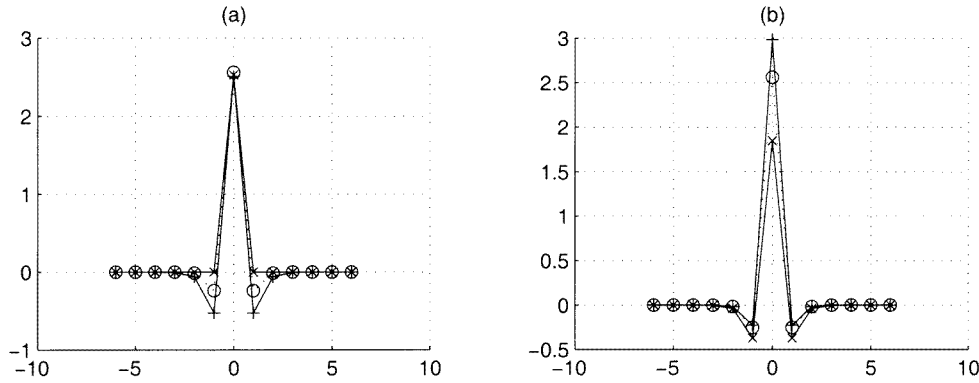


Figure 3. Initial profiles of breathers, (a) at frequency 0.6 with coupling $\alpha = 0.0$ (\times), $\alpha = 0.059$ (\circ) and $\alpha = 0.084$ ($+$); and (b) at coupling $\alpha = 0.084$ with frequency $\omega = 0.8$ (\times), $\omega = 0.52$ (\circ) and $\omega = 0.44$ ($+$).

bifurcation edge is reached more quickly. One method to do this (resulting in a so-called Euler–Newton scheme) is to generate the initial guess for the Newton–Rapshon algorithm by extrapolating along the tangent vector to the continuation curve at the last established point. Calculating this vector involves solving an extra set of coupled linear ODEs, but it is thought that the benefit of an enlarged parameter step length generally outweighs this extra computational cost [16].

5. The direction of continuation: a linear calculation

Corollary 12 shows that for each even one-site breather Θ of non-resonant period T there exists a family $\Theta_\alpha \in \Omega_{T,2}^+$, for α in a neighbourhood of 0, satisfying the continuation equation

$$F(\Theta_\alpha, \alpha) = \mathbf{0}, \tag{48}$$

with $\Theta_0 = \Theta$. In this section we describe a simple method for computing the *direction* of continuation away from Θ , that is $d\Theta_\alpha/d\alpha|_{\alpha=0} \in \Omega_{T,2}^+$, which will henceforth be denoted $\Theta' = (\chi_n)_{n \in \mathbb{Z}}$. The method has previously been used to provide the ‘predictor’ step in predictor–corrector schemes for continuation problems mentioned above [16], although we shall require only a greatly simplified version since we consider only the case $\alpha = 0$. Differentiating equation (48) with respect to α at $\alpha = 0$ yields

$$\frac{\partial F}{\partial \alpha}(\Theta, 0) + DF_\Theta \Theta' = 0. \tag{49}$$

Denoting the T -periodic even solution of the pendulum equation θ , one easily obtains the following explicit expressions,

$$\left[\frac{\partial F}{\partial \alpha}(\Theta, 0) \right]_n = \begin{cases} 2 \sin \theta & n = 0 \\ -\sin \theta & n = \pm 1 \\ 0 & |n| > 1, \end{cases} \tag{50}$$

and

$$[DF_{\Theta}\Theta']_n = \begin{cases} \ddot{\chi}_n + \cos\theta\chi_n & n = 0 \\ \ddot{\chi}_n + \frac{1}{2}(1 + \cos\theta)\chi_n & n = \pm 1 \\ \ddot{\chi}_n + \chi_n & |n| > 1. \end{cases} \quad (51)$$

So inverting DF_{Θ} to find Θ' amounts to solving an infinite set of ODEs,

$$\ddot{\chi}_0 + \cos\theta\chi_0 = -2\sin\theta \quad (52)$$

$$\ddot{\chi}_{\pm 1} + \frac{1}{2}(1 + \cos\theta)\chi_{\pm 1} = \sin\theta \quad (53)$$

$$\ddot{\chi}_n + \chi_n = 0 \quad |n| > 1, \quad (54)$$

in the space $\Omega_{T,2}^+$. Provided $T \notin 2\pi\mathbb{Z}$, equation (54) has only the trivial solution $\chi_n = 0$, so to first order the continuation leaves the $|n| > 1$ sites fixed at 0.

For the $|n| \leq 1$ equations (52), (53), the question remains how one should choose initial data $\chi_n(0) \in \mathbb{R}$, $\dot{\chi}_n(0) = 0$ in order to generate a T -periodic solution. Let $y_n(t)$ be the solution of the homogeneous problem with initial data $y_n(0) = 1$, $\dot{y}_n(0) = 0$, and $Y_n(t)$ be the particular integral of the inhomogeneous equation with initial data $Y_n(0) = \dot{Y}_n(0) = 0$. Then

$$\chi_n(t) = \chi_n(0)y_n(t) + Y_n(t) \quad (55)$$

and demanding that χ_n be periodic gives an overdetermined pair of linear equations,

$$\chi_n(0) = y_n(T)\chi_n(0) + Y_n(T) \quad (56)$$

$$0 = \dot{y}_n(T)\chi_n(0) + \dot{Y}_n(T) \quad (57)$$

for $\chi_n(0)$ in terms of the constants $y_n(T)$, $\dot{y}_n(T)$, $Y_n(T)$, $\dot{Y}_n(T)$. Equation (57) can be solved for $\chi_n(0)$, leaving (56) as a linear consistency condition for the constants. Clearly $\chi_{-1}(0) = \chi_1(0)$.

So the direction of change of the initial profile of a breather can be deduced by solving a coupled set of five second-order ODEs (the pendulum equation, and the homogeneous and inhomogeneous equations for $n = 0$ and $n = 1$), over the time interval $[0, T]$, computing the endpoint constants and solving (57). This has been done numerically using the fourth-order Runge–Kutta scheme implemented by Maple. The results are presented graphically in figure 4, a plot of $\chi_0(0)$ and $\chi_{\pm 1}(0)$ against frequency $\omega = 2\pi/T$. Note that for all ω , $\chi_0 > 0$ and $\chi_{\pm 1} < 0$, so the continuation starts by pulling the two off-central sites downwards, and the central site further upwards, as previously observed. Both χ_0 and $\chi_{\pm 1}$ appear to grow unbounded as $\omega \rightarrow 1$ (the small-amplitude limit) in agreement with the observation that the length of the continuation neighbourhood vanishes in this limit. The graph suggests that as $\omega \rightarrow 0$ ($T \rightarrow \infty$), χ_0 vanishes, while $\chi_{\pm 1}$ tends to a non-zero constant. Of course, this limit is numerically inaccessible, so these remarks are necessarily speculative. One can estimate $\chi_n(0)$ from the numerical work of section 4 by comparing Θ with Θ_{α} after the first continuation step. The results of this calculation are also presented in figure 4 (broken curve) for purposes of comparison with the linear method.

6. Conclusion

In this paper we have adapted the methods of MacKay and Aubry to prove existence of breathers in the TDSG system, despite the fact that there is no limit in which the system decouples into independent oscillators (so the existence theorems so far formulated [1, 2] do

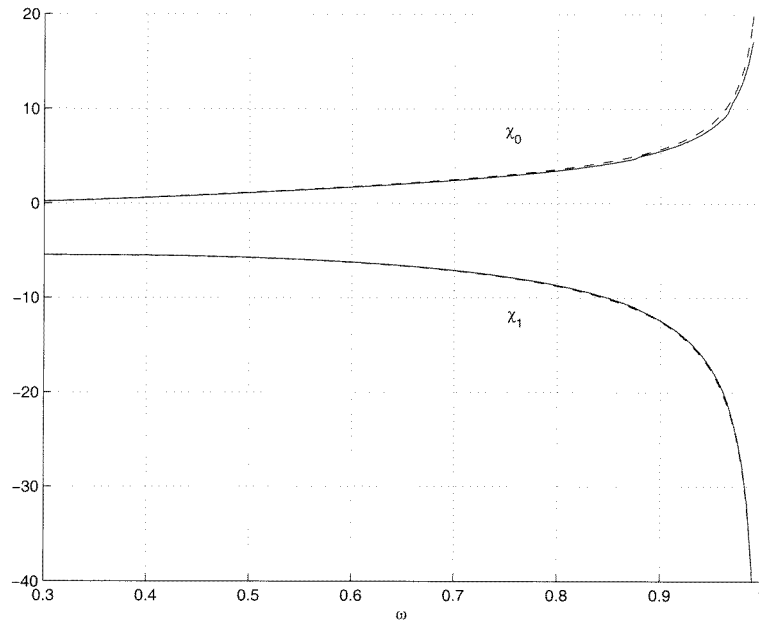


Figure 4. The components χ_0 and χ_1 of the tangent vector Θ' as functions of frequency, ω . The full curves were generated using the linear method, the broken curves from the breather profiles generated by the numerical scheme described in section 4. The two data sets agree closely (especially for χ_1).

not directly apply). Numerical analysis has revealed that the persistence of these breathers away from the $h = 2$ limit depends critically on their period. One reason for this is that the coupling at which the breather enters into resonance with the phonons depends on its frequency. However, for most frequencies the continuation actually fails before it reaches the phonon resonance region. The underlying mechanism for these early bifurcations is at present unknown. A full bifurcation analysis may prove informative.

In no case does existence persist for all $h \in (0, 2]$, so the breathers found here are unconnected with the breathers of the continuum sine-Gordon system (which the TDSG system approaches as $h \rightarrow 0$). Indeed, they look qualitatively different from continuum breathers in that they have sombrero rather than hump-shaped initial profiles. In this respect they appear to differ also from breathers found in previous studies of spatially discrete systems. By means of a simple linear method, we have confirmed the uniform trend towards sombrero-shaped breathers in the TDSG system. It would be interesting to apply the same linear method to a variety of more conventional oscillator networks, since this allows one to examine the direction of continuation of one-site breathers away from the weak coupling limit with a minimum of computational effort.

Acknowledgments

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Appendix

The proof of invertibility of DF_Θ rested on the following lemma, whose proof we now give.

Proof of lemma 4. Each of the difference equations (35)–(37) is of a type subject to the following theorem of Poincaré [17].

Theorem 13 (Poincaré). *Let f_1, f_2 be functions with limits p_1, p_2 respectively as $n \rightarrow \infty$, such that the polynomial $P(\lambda) = \lambda^2 + p_1\lambda + p_2$ has two distinct real roots λ_1, λ_2 . Then any solution of the linear second-order difference equation $y_{n+1} + f_1(n)y_n + f_2(n)y_{n-1} = 0$ has the asymptotic behaviour $\lim_{n \rightarrow \infty} \frac{y_{n+1}}{y_n} = \lambda_i$ for either $i = 1$ or $i = 2$.*

In each of the three cases of interest here, P is the same polynomial, namely $P(\lambda) = \lambda^2 + \frac{2}{a}\lambda + 1$. For $a \in (0, 1)$, this has two distinct negative roots whose product is unity. Let λ_1 denote the larger root, so that $|\lambda_1| < 1$ while $|\lambda_2| > 1$. To prove exponential divergence of A^σ , $\sigma = 1, 2, 3$, it is convenient to define the quotient sequences

$$B_n^\sigma = -\frac{A_{n+1}^\sigma}{A_n^\sigma}, \tag{58}$$

which satisfy first-order nonlinear recurrence relations. Note that the sequence B^σ exists if and only if it never vanishes. We will assume that these sequences exist, and justify the assumption *a posteriori*. By Poincaré’s theorem, for each σ the sequence $B^\sigma \rightarrow |\lambda_i|$ for either $i = 1$ or $i = 2$. To prove exponential divergence of A^σ therefore, it suffices to show that B^σ cannot converge to a limit less than 1.

Part (a). From the difference equation (35), one finds that B^1 satisfies the first-order recurrence relation

$$B_n^1 = \frac{4n^2 - 4n + a}{a(2n - 1)(n + 1)} - \frac{n - 2}{n + 1} \frac{1}{B_{n-1}^1} \tag{59}$$

with initial condition $B_1^1 = 1$. We claim that $B_n^1 \geq 1$ for all $n \in \mathbb{N}$. The proof is by induction. Assume $B_{n-1}^1 \geq 1$. Then

$$\begin{aligned} B_n^1 &= \frac{4n^2 - 4n}{a(2n - 1)(n + 1)} + \frac{1}{(2n - 1)(n + 1)} - \frac{n - 2}{n + 1} \frac{1}{B_{n-1}^1} \\ &> \frac{4n^2 - 4n + 1}{(2n - 1)(n + 1)} - \frac{n - 2}{n + 1} = 1. \end{aligned} \tag{60}$$

Since $B_n^1 \geq 1$ for all $n \in \mathbb{N}$, the sequence exists (never vanishes) and cannot converge to $|\lambda_1| < 1$. Hence $B^1 \rightarrow |\lambda_2| > 1$, and A^1 is exponentially divergent.

Part (b). From the difference equation (36), one finds that B^2 satisfies the first-order recurrence relation

$$B_n^2 = \frac{8}{a} \frac{n(n - 1)}{4n^2 + 2n - 1} - \frac{4n^2 - 10n + 5}{4n^2 + 2n - 1} \frac{1}{B_{n-1}^2} \tag{61}$$

with initial condition $B_1^2 = \frac{1}{5}$. Since the solution of (61) depends on the parameter a we will denote it $B^2(a)$, and further, allow a to take all values in $(0, 1]$, denoting $B^2(1)$ by \bar{B} . The first step is to prove that \bar{B} exists (is non-vanishing) and does not converge to a limit less than 1. Assume $\bar{B}_{n-1} > n/(n + 1)$. Then for all $n \geq 2$

$$\bar{B}_n - \frac{n + 1}{n + 2} > \frac{8n(n - 1)}{4n^2 + 2n - 1} - \frac{4n^2 - 10n + 5}{4n^2 + 2n - 1} \frac{n + 1}{n} = \frac{6n - 10}{(4n^2 + 2n - 1)(n + 2)n} > 0. \tag{62}$$

Explicit evaluation of the first few terms yields that $\bar{B}_3 = \frac{37}{41} > \frac{4}{5}$. Hence, by induction, for all $n \geq 3$, $\bar{B}_n > (n+1)/(n+2)$, so \bar{B} exists and does not converge to a limit less than 1. Now consider the sequence $B^2(a)$ for $a < 1$. We claim that each term $B_n^2(a)$ is a non-increasing function on $(0, 1]$. To see this, observe that $B_1^2(a) = \frac{1}{5}$ is manifestly non-increasing, and assume that $B_{n-1}^2(a)$ is non-increasing for some $n \geq 2$. Then $B_{n-1}^2(a) \geq B_{n-1}^2(1) = \bar{B}_{n-1} > 0$ by the paragraph above, so $B_{n-1}^2(a)$ is positive and non-increasing. From relation (61) it immediately follows that $B_n^2(a)$ is non-increasing, so the claim is proved. Hence $B^2(a)$ is strictly positive (and hence exists) for all $a \in (0, 1)$. Further $\lim B^2(a) \geq \lim \bar{B} \geq 1 > |\lambda_1|$, so $B^2 \rightarrow |\lambda_2|$ and A^2 is exponentially divergent.

Part (c). The argument is almost identical to part (b). The sequence $B^3(a)$ satisfies

$$B_n^3 = \frac{2}{a} \frac{4n^2 - 1}{4n^2 + 6n + 1} - \frac{4n^2 - 6n + 1}{4n^2 + 6n + 1} \frac{1}{B_{n-1}^3} \quad (63)$$

with initial condition $B_1^3(a) = \frac{6}{11a}$. Once again we allow a to take all values in $(0, 1]$ and denote $B^3(1)$ by \bar{B} . We claim that for all $n \in \mathbb{N}$, $\bar{B}_n > n/(n+1)$. Clearly, the claim holds true for $n = 1$. Assume $\bar{B}_{n-1} > (n-1)/n$ for some $n \geq 2$. Then

$$\begin{aligned} \bar{B}_n &> 2 \frac{4n^2 - 1}{4n^2 + 6n + 1} - \frac{4n^2 - 6n + 1}{4n^2 + 6n + 1} \frac{n}{n-1} \\ &\Rightarrow \bar{B}_n - \frac{n}{n+1} > \frac{2}{(4n^2 + 6n + 1)(n+1)(n-1)} > 0, \end{aligned} \quad (64)$$

so that $\bar{B}_n > n/(n+1)$ and the claim is proved. Hence \bar{B} is strictly positive (hence exists) and cannot converge to a limit less than 1.

We next claim that for each $n \in \mathbb{N}$, $B_n^3(a)$ is a decreasing function on $(0, 1]$. Clearly $B_1^3(a) = \frac{6}{11a}$ is decreasing. Assume that $B_{n-1}^3(a)$ is decreasing. Then $B_{n-1}^3(a) \geq B_{n-1}^3(1) = \bar{B}_{n-1} > 0$, so B_{n-1}^3 is a positive decreasing function of a . It follows from (63) that $B_n^3(a)$ is also decreasing, and the claim is proved. Hence $B^3(a)$ is strictly positive (and hence exists) for all $a \in (0, 1)$. Further $\lim B^3(a) \geq \lim \bar{B} \geq 1 > |\lambda_1|$, so $B^3 \rightarrow |\lambda_2|$ and A^3 is exponentially divergent. \square

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