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Stationary breather modes of generalized nonlinear Klein–Gordon lattices

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Abstract. This paper studies the form of stationary breather modes in discrete generalized nonlinear Klein–Gordon equations, with symmetric and non-symmetric potential energy functions. In the case of static breathers, the discrete nature of the spatial dimension has a much more subtle effect on the breather than the moving breather mode. This effect is analysed using a variety of approximating partial differential equations, whose solutions are found by using an extended multiple-scales asymptotic approach to reduce the equation to a nonlinear Schrödinger equation at leading order and more complex equations at higher order, where secularity conditions are required to fully specify the solution. As well as the much studied discrete sine–Gordon equation, the methods are demonstrated on a discrete nonlinear Klein–Gordon equation with second-neighbour interactions and non-symmetric on-site potential. New partial differential equations which approximate these lattice systems are also proposed and analysed.

1. Introduction

The existence of breathers in the discrete sine–Gordon equation has been proven by MacKay and Aubry [6] and more recently some 'practical' stability results have been derived by Bambusi [1]. However, Konwent *et al* [5] have shown that modified systems can have different properties and exhibit less straightforward behaviour.

The differences between breathers in the sine–Gordon (SG) and discrete sine–Gordon systems (DSG) were explored by Remoissenet [7]. In that paper a leading-order asymptotic expansion was used to analyse moving breathers and the results applied to a specific example. Here we shall study stationary breathers. Larger amplitude breathers in the DSG system are observed to be pinned to a lattice site, it is only small amplitude breathers which move freely through the lattice. This has been observed in the numerical work of Dauxois and Peyrard [2], and some analytical work has started to elucidate the reasons for this pinning [14]. To understand this pinning effect it is important to know in what ways a discrete spatial dimension affects a breather's properties.

Hence it is of interest to find the difference in shape between breathers in continuous and discrete systems. The work of Remoissenet [7] shows no difference between the two for static breathers, since in this case the differences occur at a higher order than for moving breathers. The aim of this paper is to perform the asymptotic reduction of the equation for stationary breathers to a higher order to find the difference in shape.

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The results are applied to an example system of a coupled pair of chains, each of which has nearest-neighbour and second-neighbour interactions. The chains considered are parallel to each other, connected by nonlinear springs and a new interaction—that of diagonal linear springs. To analyse the system's dynamics, a transformation is used which uncouples the equations into a linear differential-difference equation and a discrete nonlinear Klein–Gordon system with second-neighbour interactions. This latter problem—an infinite set of ordinary differential equations—is approximated by a variety of partial differential equations, and ultimately solved using multiple-scales techniques to give a breather solution which has a component caused specifically by the the discrete nature of the underlying system. Higher-order, multiple-scales methods require the use of secularity conditions to solve a hierarchy of equations generated by higher-order, multiple-scales analysis.

A variety of possible partial differential equations (PDEs) approximating the system of ordinary differential equations are suggested. These are generated using function theoretic methods which have successfully been applied to lattices of Fermi–Pasta–Ulam (FPU) type. For each approximating equation a dispersion relation is calculated to show how accurately (or otherwise) the equation replicates the response of the lattice to small-amplitude linear waves.

The remainder of this section introduces the systems studied and some of their basic properties. In section 2 we show how to form new approximate PDEs which imitate the behaviour of the DSG system. Section 3 shows that breather solutions can be found for these systems, which correspond to breather solutions for the DSG system. The second part of this paper applies these methods to a more general nonlinear Klein–Gordon lattice: in section 4 a variety of PDEs are derived which approximate the lattice; and the solution is derived in section 5. Finally, a discussion of our results is given in section 6.

1.1. Derivation of the DSG equation

The DSG equation can be derived from the Hamiltonian

$$H = \sum_n \tfrac{1}{2}\dot{\phi}_n^2 + \tfrac{1}{2}(\phi_{n+1} - \phi_n)^2 + \Gamma^2(1 - \cos\phi_n) \tag{1.1}$$

which models a lattice of particles with positions $\phi_n(t)$ each interacting with its nearest neighbour via a linear spring and each experiencing a nonlinear 'on-site' potential with energy $\Gamma^2(1 - \cos\phi_n)$. Thus the equations of motion are

$$\ddot{\phi}_n = \phi_{n+1} - 2\phi_n + \phi_{n-1} - \Gamma^2 \sin\phi_n. \tag{1.2}$$

This system of ordinary differential equations has received much study, since it occurs naturally as a model for many physical processes where the underlying spatial structure is inherently discrete. Its continuum counterpart, the SG equation

$$\frac{\partial^2\phi}{\partial t^2} = \frac{\partial^2\phi}{\partial x^2} - \Gamma^2 \sin\phi \tag{1.3}$$

is an integrable system and can be derived from the Hamiltonian density $\mathcal{H} = \frac{1}{2}\phi_t^2 + \frac{1}{2}\phi_x^2 + \Gamma^2(1 - \cos\phi)$. Both the SG and DSG equations are widely studied, but the discrete equation (1.2) is not integrable and thus many of the mathematical tools used in the study of the SG equation (1.3) are not available to those wishing to analyse the effects that the discrete nature of the spatial dimension has on the kinetics of (1.2).

If we look at the behaviour of small amplitude linear waves in each of these systems, we find some of the differences between continuum and discrete equations. Substituting a wave of the form $\phi_n(t) = \varepsilon \exp \mathrm{i}(kn - \omega t)$, with $\varepsilon \ll 1$, then we find that in the DSG equation

$$\omega_{\mathrm{DSG}}^2 = \Gamma^2 + 4\sin^2(\tfrac{1}{2}k) \tag{1.4}$$

whereas for the continuous SG equation

$$\omega_{\mathrm{SG}}^2 = \Gamma^2 + k^2. \tag{1.5}$$

The continuous case has a minimum frequency, but no maximum, whereas the discrete equation has a finite band of frequencies: ω must lie between Γ and $\sqrt{(\Gamma^2+4)}$.

If we replace the discrete spatial variable n by the continuous variable x and then expand δ_n^2, the centred second spatial difference of (1.2) in a Taylor series, we find $\delta_n^2 = \partial_x^2 + \frac{1}{12}\partial_x^4 + \cdots$, and hence obtain the equation

$$\phi_{tt} - \phi_{xx} - \tfrac{1}{12}\phi_{xxxx} - \cdots + \Gamma^2 \sin\phi = 0. \tag{1.6}$$

Rescaling the independent variables with Γ, by $\tau = \Gamma t$, $\xi = \Gamma x$, leads to the equation

$$\phi_{\tau\tau} - \phi_{\xi\xi} + \sin\phi = \tfrac{1}{12}\Gamma^2\phi_{\xi\xi\xi\xi} + \mathrm{O}(\Gamma^4). \tag{1.7}$$

So, in the limit $\Gamma \to 0$, the SG equation is approached. However, for any $\Gamma > 0$, there is always a value of k so large that ω_{SG} is larger than the maximum frequency allowed in the DSG equation. In a later section, we shall show that it is possible to construct partial differential equations which approximate the DSG equation, and also have the behaviour that linear waves only occupy a finite band of frequencies.

1.2. Generalized Klein–Gordon lattice

We shall also study a lattice system which comes from modelling two coupled chains of atoms. The lattice we consider is a generalization of a model for DNA.

We assume that each atom on each chain has harmonic interactions with its nearest neighbours and with its second neighbours on the same chain. At rest, atoms are spaced equidistantly along each chain, with the same spacing on each chain. The chains are parallel and coupled by both linear and nonlinear springs; an atom in the first chain has a nonlinear interaction with a corresponding atom in the other chain, and a linear interaction with the atom either side of this—a diagonal interaction. This is perhaps more clearly seen in figure 1, where the coils represent linear springs, and the hollow rectangles mark the nonlinear springs. In forming kinetic equations for the motion of such a lattice, we assume that all atoms have unit mass, and the spring constant for nearest-neighbour interactions is f, whilst that for second neighbours is g and for the diagonal interactions h. The energy stored in the nonlinear springs will be denoted by the function $V(x_n - y_n)$, where the displacements of atoms on the chains is given by x_n, y_n. In general, $V(\phi)$ will not be an even function, and since our analysis does not rely on any numerical work, no assumptions will be made on the form of V other than that it possesses a Taylor series.

The Hamiltonian is then

$$H = \sum_n \tfrac{1}{2}\dot{x}_n^2 + \tfrac{1}{2}\dot{y}_n^2 + \tfrac{1}{2}f(x_{n+1}-x_n)^2 + \tfrac{1}{2}f(y_{n+1}-y_n)^2 + \tfrac{1}{2}g(x_{n+2}-x_n)^2 + \tfrac{1}{2}g(y_{n+2}-y_n)^2 + \tfrac{1}{2}h(y_{n+1}-x_n)^2 + \tfrac{1}{2}h(x_{n+1}-y_n)^2 + V(x_n-y_n) \tag{1.8}$$

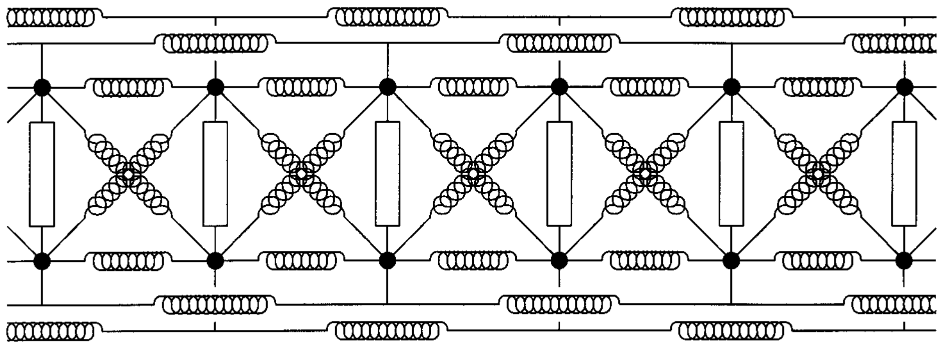

Figure 1. A diagram showing connectivity of the lattice chain under consideration. Each bullet point represents a node and boxes represent nonlinear springs, all other connections being linear springs.

which generates the equations of motion

$$\ddot{x}_n = f(x_{n+1} - 2x_n + x_{n-1}) + g(x_{n+2} - 2x_n + x_{n-2}) + h(y_{n+1} - 2x_n + y_{n-1}) - V'(x_n - y_n)$$
$$\ddot{y}_n = f(y_{n+1} - 2y_n + y_{n-1}) + g(y_{n+2} - 2y_n + y_{n-2}) + h(x_{n+1} - 2y_n + x_{n-1}) + V'(x_n - y_n). \tag{1.9}$$

The transformation $\psi_n = x_n + y_n$, $\phi_n = x_n - y_n$ enables these two equations to be separated into a linear equation for the summed displacements and a nonlinear Klein–Gordon equation with second-neighbour interactions for the differences in displacements of the two chains:

$$\ddot{\psi}_n = (f + h)(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + g(\psi_{n+2} - 2\psi_n + \psi_{n-2})$$
$$\ddot{\phi}_n = (f - h)(\phi_{n+1} - 2\phi_n + \phi_{n-1}) + g(\phi_{n+2} - 2\phi_n + \phi_{n-2}) - 2V'(\phi_n) - 4h\phi_n. \tag{1.10}$$

Thus the effect of the springs forming diagonal connections can be removed by redefining the nearest-neighbour interaction spring constants, and making a minor modification to the nonlinear interaction potential $V(\phi)$. We shall assume that for small-amplitude disturbances, $2V'(\phi) + 4h\phi \sim \Gamma^2\phi +$ higher-order terms.

We need to analyse the dispersion relations to see what values of f, g, h and Γ are allowable. Since the equation for ψ_n is linear, we assume a travelling-wave solution of the form $\psi_n = e^{i(kn-\omega t)}$. The dispersion relation is then

$$\omega_\psi^2 = 4(f + h + 4g\cos^2(\tfrac{1}{2}k))\sin^2(\tfrac{1}{2}k). \tag{1.11}$$

Thus for stability of the zero-solution ground state, we require $h + f > 0$ (from $k = \pi$) and $h + f + 4g > 0$ (from $k \to 0$). These are entirely reasonable conditions since in most physical systems we would expect nearest-neighbour interactions to be stronger than second-neighbour or diagonal interactions.

The dispersion relation for ϕ is

$$\omega_\phi^2 = \Gamma^2 + 4(f - h + 4g)\sin^2(\tfrac{1}{2}k) - 16g\sin^4(\tfrac{1}{2}k). \tag{1.12}$$

From $k = \pi/2$ we get the requirement $f - h > -\frac{1}{4}\Gamma^2$. The dispersion relation gives real frequencies for all $g > -\frac{1}{4}|f - h|$. (For certain combinations of parameter values outside this limit the equation is still well-posed.)

This model opens up the possibility of a new form of discrete Klein–Gordon equation, where the central difference term has the opposite sign from that expected in continuum systems. For example, if we take $g = 0$, $h = 1$, and $f = 0$ then the equation for ψ is well-posed, and the dispersion relation for ϕ implies that we need $V''(0) > 0$ for well-posedness. However, the resulting equation

$$\ddot{\phi}_n = -\phi_{n+1} + 2\phi_n - \phi_{n-1} - V'(\phi_n) \tag{1.13}$$

has no obvious well-posed continuum approximation.

For simplicity let us consider the case where $V'(\phi)$ is an odd function; we make the substitution $\eta_n = (-1)^n\phi_n$, to obtain

$$\ddot{\eta}_n = \eta_{n+1} - 2\eta_n + \eta_{n-1} - V'(\eta_n) + 4\eta_n \tag{1.14}$$

which has the dispersion relation $\omega_\eta^2 = V''(0) - 4 + 4\sin^2\left(\frac{1}{2}k\right)$, so that provided $V''(0) > 4$ the PDE is well-posed. A continuum approximation of the equation is possible

$$\frac{\partial^2\eta}{\partial t^2} = \frac{\partial^2\eta}{\partial x^2} - V'(\eta) + 4\eta \tag{1.15}$$

which also has a well defined dispersion relation $\omega_{\eta,\mathrm{cts}}^2 = V''(0) - 4 + k^2$, with exactly the same condition on well-posedness. Thus, in cases where the sign of the spatial difference is reversed, there are solutions which are similar to breathers, but where adjacent atoms have displacements in opposite directions.

2. PDE approximations to the DSG system

In this section we derive new partial differential equations which approximate the DSG system. The similarities and differences between the approximations and the fully discrete system will be outlined, particularly in the behaviour of linear waves in these systems. In the next section, we shall show how breather solutions are found from the approximations.

We exploit the technique used in earlier papers where the second difference operator is approximated using ratios of polynomials—a technique also known as Padé approximation. Here, however, instead of forming expansions in terms of the ratio of two polynomials in a variable, the polynomials will be functions of the differential operator, $\partial_x := \partial/\partial x$. Identical results can be obtained by taking the Fourier transform in x, then performing a Padé approximation of a function in terms of the transform variable before inverting the transform. The method presented here simply requires less manipulation. Such a technique was used successfully in approximating the travelling-wave solution of the FPU chain [3, 10], the chain with second-neighbour interactions [12], and a two-dimensional lattice [11].

Various forms of continuum approximations are open to us, although only the standard SG equation is second order. All the new approximations take the form of higher-order PDEs. We have already noted that the dispersion relation for this equation is significantly different to that for the DSG equation. There are three approximations which lead to fourth-order PDEs described here, all based on Padé approximations of the centred second difference operator.

2.1. (4,0) Padé approximation

This is the simplest of the three, and really only a Taylor approximation of the difference operator $\delta_n^2 \sim \partial_x^2 + \frac{1}{12}\partial_x^4$. The partial differential equation it generates is

$$\phi_{tt} - \phi_{xx} + \Gamma^2\sin\phi = \tfrac{1}{12}\phi_{xxxx} \tag{2.1}$$

with dispersion relation

$$\omega^2 = \Gamma^2 + k^2 - \tfrac{1}{12}k^4. \tag{2.2}$$

This has a minimum at $k = 0$ and a maximum (at $k = \sqrt{6}$)—qualitatively the same as the DSG equation which rises to a maximum at $k = \pi$; but for values of k above $\sqrt{6}$, the dispersion relation (2.2) decreases through zero, and becomes negative. Thus the zero solution of the partial differential equation (2.1) is unstable to high-frequency perturbations—in this respect it is not a good approximation of the lattice.

Equation (2.1) can be derived from a Lagrangian or Hamiltonian ($\mathcal{L} = \frac{1}{2}\phi_t^2 + \frac{1}{2}\phi_x^2 - \frac{1}{24}\phi_{xx}^2 - \Gamma^2(1-\cos\phi)$).

2.2. (2,2) Padé approximation

Here the difference operator is approximated by $\delta_n^2 \sim (1 - \frac{1}{12}\partial^2)^{-1}\partial_x^2$, which generates the partial differential equation

$$\phi_{tt} = \phi_{xx} - \Gamma^2 \sin\phi + \tfrac{1}{12}\phi_{xxtt} + \tfrac{1}{12}\Gamma^2(\phi_{xx}\cos\phi - \phi_x^2 \sin\phi). \tag{2.3}$$

Although the DSG system is Lagrangian, and the (4,0) Padé approximation has a Lagrangian structure, no Lagrangian has been found for this equation. The dispersion relation for (2.3) is

$$\omega^2 = \frac{\Gamma^2 + k^2 + \frac{1}{12}\Gamma^2 k^2}{1 + \frac{1}{12}k^2}. \tag{2.4}$$

This remains positive for all values of k, has a minimum at $k = 0$ (of $\omega = \Gamma$) and a maximum as $k \to \infty$ (where $\omega \to \sqrt{(\Gamma^2 + 12)}$). Thus this has the right physical properties of a finite band of linear frequency modes and shows the stability of the zero solution.

2.3. (4,2) Padé approximation

This approximation

$$\delta_n^2 \sim \left[\frac{1 + \frac{1}{20}\partial_x^2}{1 - \frac{1}{30}\partial_x^2}\right]\partial_x^2 + \mathrm{O}(\partial_x^8) \tag{2.5}$$

is sixth order accurate in ∂_x, yet still provides a fourth-order PDE

$$\phi_{tt} = \phi_{xx} - \Gamma^2 \sin\phi + \tfrac{1}{20}\phi_{xxxx} + \tfrac{1}{30}\phi_{xxtt} + \tfrac{1}{30}\Gamma^2(\phi_{xx}\cos\phi - \phi_x^2 \sin\phi). \tag{2.6}$$

As for the (2,2) Padé approximation, no Lagrangian has been found for this case. The dispersion relation for (2.6) is

$$\omega^2 = \frac{\Gamma^2 + k^2 - \frac{1}{20}k^4 + \frac{1}{30}\Gamma^2 k^2}{1 + \frac{1}{30}k^2} \tag{2.7}$$

which becomes negative for large k, demonstrating unphysical behaviour in that the zero solution is unstable to linear modes with high wavenumbers. For smaller k, (2.7) will give a better approximation to the shape of the DSG dispersion relation. It has a maximum at $k = \sqrt{10(\sqrt{15} - 3)} \approx 2.9546$ where $\omega = \sqrt{\Gamma^2 + 120 - 2\sqrt{15}} \approx \sqrt{\Gamma^2 + 10.595^2}$.

Figure 2 shows dispersion relations for the various approximations to the DSG equation which are developed above. All give accurate representations for small k, but none are accurate as far as $k = \pm 2\pi$. Both (4,2) and (4,0) Padé approximations give an indication of the existence of a local maximum in the frequency, but neither manage to get to $k = \pm 2\pi$ without giving complex frequencies—indicating that the partial differential equations are ill-posed in the sense that arbitrarily small linear waves grow in amplitude. The (2,0) Padé approximation is inaccurate in that it allows arbitrarily large frequencies for linear modes

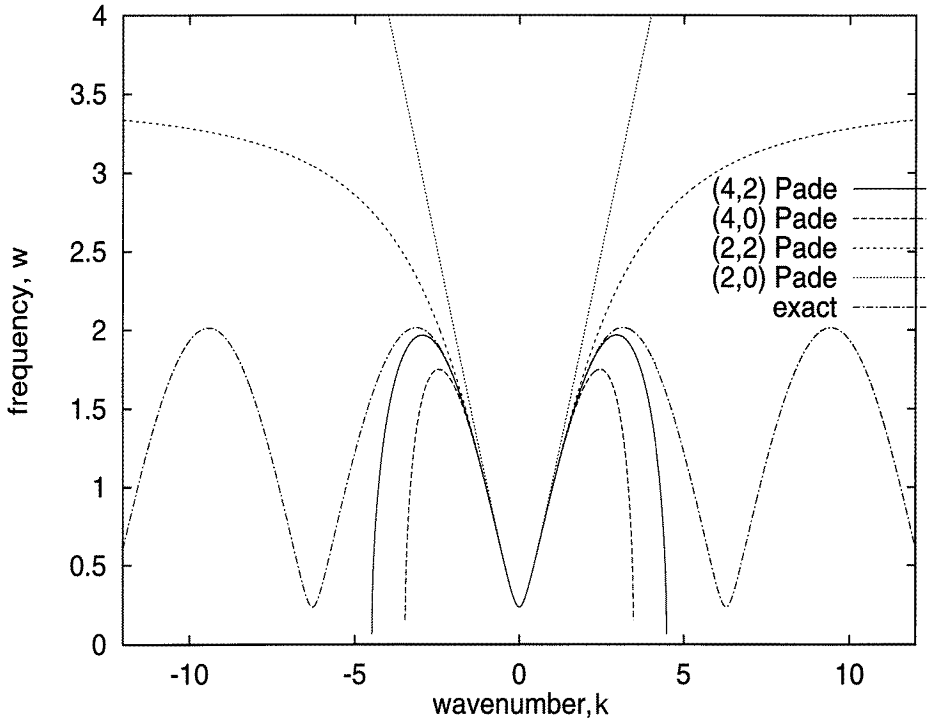

Figure 2. The dispersion relation for DSG and each approximation to the DSG equation (with $\Gamma = 0.236$).

with large wavenumber. Only the (2,2) Padé approximate predicts that all waves should have frequencies lying within a band of finite width. In the example shown above, the lattice allows $0.236 \leqslant \omega \leqslant 2.01$, whereas the (2,2) Padé approximate predicts $0.236 \leqslant \omega \leqslant 3.47$. However, the periodicity in wavenumber is not well captured, as the (2,2) approximate is monotonic in $k > 0$.

3. Static breather solutions of the DSG equation

Having found a variety of PDEs which approximate the DSG equation to varying degrees of accuracy, we aim to use these to find breather solutions. This will be performed by using the method of multiple scales from asymptotic analysis. It will be necessary to carry this out beyond leading order in order to find the effects of discreteness. The leading-order analysis is commonly used, but to obtain a description of the more subtle aspects of behaviour higher-order terms are required, and to find these, secularity conditions need to be found and solved. So although the end results appear straightforward, the analysis leading to them is non-trivial. Details of the procedure will be explained as encountered.

3.1. Solution to the (4,0) Padé equation

The essence of the method of multiple scales is to expand the dependent variable in terms of an asymptotic series, whilst the independent variable(s) are replaced by a hierarchy of 'slow' variables. Since the PDEs we are interested in have two independent variables (x and t), we have two hierarchies of slow variables.

Knowing the form of the solution of the purely continuum SG case enables us to reduce the number of terms we have to consider. The hierarchies of new independent variables replacing x and t are

$$\begin{array}{llll} t_0 = t & t_2 = \varepsilon^2 t & t_4 = \varepsilon^4 t & \ldots \\ x_1 = \varepsilon x & x_3 = \varepsilon^3 x & \ldots & \end{array} \tag{3.1}$$

so that the x- and t-derivatives are replaced by

$$\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial}{\partial t_0} + \varepsilon^2 \frac{\partial}{\partial t_2} + \varepsilon^4 \frac{\partial}{\partial t_4} + \cdots \\ \frac{\partial}{\partial x} &= \varepsilon \frac{\partial}{\partial x_1} + \varepsilon^3 \frac{\partial}{\partial x_3} + \cdots . \end{aligned} \tag{3.2}$$

Next, we specify the asymptotic series for ϕ; we make the ansatz that the solution is of the form

$$\begin{aligned} \phi = \varepsilon\, \mathrm{e}^{\mathrm{i}\Gamma t_0} F_1(x_1, t_2, x_3, t_4) &+ \varepsilon^3 [\mathrm{e}^{\mathrm{i}\Gamma t_0} F_3(x_1, t_2) + \mathrm{e}^{3\mathrm{i}\Gamma t_0} G_3(x_1, t_2)] \\ &+ \varepsilon^5 [\mathrm{e}^{\mathrm{i}\Gamma t_0} F_5(x_1, t_2) + \mathrm{e}^{3\mathrm{i}\Gamma t_0} G_5(x_1, t_2) + \mathrm{e}^{5\mathrm{i}\Gamma t_0} H_5(x_1, t_2)] + \cdots + \mathrm{CC}. \end{aligned} \tag{3.3}$$

This solution ansatz, together with the multiple-scales expansion (3.2) is substituted into a small-amplitude expansion of the PDE (2.1)

$$\phi_{tt} = -\Gamma^2 \phi + \tfrac{1}{6} \Gamma^2 \phi^3 - \tfrac{1}{120} \Gamma^2 \phi^5 + \phi_{xx} + \tfrac{1}{12} \kappa \phi_{xxxx} \tag{3.4}$$

to find an equation which contains terms in a variety of orders of ε each with a certain frequency in the $\mathcal{O}(1)$ timescale, t_0. The extra constant κ has been inserted in front of the term which is present in an expansion of the DSG equation, but absent from an expansion of the SG equation. This will ease interpretation of the results at a later stage. In the ensuing analysis we are thus solving two systems: $\kappa = 1$ corresponds to the DSG equation and $\kappa = 0$ to the SG equation.

We obtain six equations from (3.4) by equating the coefficients of each harmonic frequency at each order of ε

$\mathcal{O}(\varepsilon^3\, \mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$2\mathrm{i}\Gamma F_{1,t_2} - \Gamma^2 F_3 = -\Gamma^2 F_3 + \tfrac{1}{2}\Gamma^2 |F_1|^2 F_1 + F_{1,x_1x_1}$$

$\mathcal{O}(\varepsilon^3\, \mathrm{e}^{3\mathrm{i}\Gamma t_0})$:

$$-9\Gamma^2 G_3 = -\Gamma^2 G_3 + \tfrac{1}{6}\Gamma^2 F_1^3$$

$\mathcal{O}(\varepsilon^5\, \mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$\begin{aligned} 2\mathrm{i}\Gamma F_{1,t_4} + F_{1,t_2t_2} + 2\mathrm{i}\Gamma F_{3,t_2} - \Gamma^2 F_5 &= -\Gamma^2 F_5 + \tfrac{1}{2}\Gamma^2 F_1^2 \bar{F}_3 + \Gamma^2 |F_1|^2 F_3 \\ &\quad + \tfrac{1}{2}\Gamma^2 \bar{F}_1^2 G_3 + \tfrac{1}{12}\Gamma^2 |F_1|^4 F_1 + F_{3,x_1x_1} + 2F_{1,x_1x_3} + \tfrac{1}{12}\kappa F_{1,x_1x_1x_1x_1} \end{aligned}$$

$\mathcal{O}(\varepsilon^5\, \mathrm{e}^{3\mathrm{i}\Gamma t_0})$:

$$6\mathrm{i}\Gamma G_{3,t_2} - 9\Gamma^2 G_5 = -\Gamma^2 G_5 + \tfrac{1}{2}\Gamma^2 F_1^2 F_3 + \Gamma^2 |F_1|^2 G_3 + \tfrac{1}{24}\Gamma^2 |F_1|^2 F_1^3 + G_{3,x_1x_1}$$

$\mathcal{O}(\varepsilon^5\, \mathrm{e}^{5\mathrm{i}\Gamma t_0})$:

$$-25\Gamma^2 H_5 = -\Gamma^2 H_5 + \tfrac{1}{2}\Gamma^2 F_1^2 G_3 + \tfrac{1}{120}\Gamma^2 F_1^5. \tag{3.5}$$

The equation obtained by considering $\mathcal{O}(\varepsilon\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ terms is automatically satisfied; the first equation displayed above (from $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ terms) is the nonlinear Schrödinger (NLS) equation. The solution we are interested in is

$$F_1 = A\,\mathrm{e}^{\mathrm{i}\Omega}\,\mathrm{e}^{-\mathrm{i}\Gamma A^2 t_2/8}\mathrm{sech}(\tfrac{1}{2}\Gamma A x_1 + B) \tag{3.6}$$

where A, B and Ω are real constants of integration which may depend on x_3 and t_4. Since this expression contains no κ term, there is no difference at $\mathcal{O}(\varepsilon)$ between the SG and DSG breather modes.

We specify that the amplitude of the breather is $\phi(0,0) = 2\varepsilon A$ exactly; i.e. the corrections we calculate at the next order will change the shape and temporal behaviour of the breather, but not alter its amplitude. Thus $F_3(0,0,0,0) + G_3(0,0,0,0) = 0$.

The equation from the $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$ terms is interpreted as an algebraic equation for G_3 and has the solution $G_3 = -\frac{1}{48}F_1^3$. We shall pass over the equation for F_3 from $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ terms for now, and return to it later; however, we will assume that its solution can be found so that later equations can be solved in terms of F_3. Solving this equation is the crux of our analysis.

The equation derived from $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$ terms is another algebraic equation, this time for G_5

$$G_5 = \frac{1}{64\Gamma^2}(F_1 F_{1,x_1}^2 - F_1^2 F_{1,x_1x_1}) - \frac{1}{96}F_1^2 F_3 - \frac{1}{256}|F_1|^2 F_1^3. \tag{3.7}$$

Finally, from consideration of $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{5\mathrm{i}\Gamma t_0})$ terms, we find $H_5 = \frac{1}{1280}F_1^5$.

In this brief run-through of the equations, we ignored terms of $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$—a much more complicated equation. Although coming from an $\mathcal{O}(\varepsilon^5)$ part of the DSG expansion, the equation actually determines the $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ correction to ϕ, namely F_3. Using the solution we have already found for G_3, the equation can be simplified to

$$\begin{aligned}2\mathrm{i}\Gamma F_{3,t_2} - F_{3,x_1x_1} - \tfrac{1}{2}\Gamma^2 F_1^2 \bar{F}_3 - \Gamma^2|F_1|^2 F_3 = 2F_{1,x_1x_3} - F_{1,t_2t_2} - 2\mathrm{i}\Gamma F_{1,t_4}\\ + \tfrac{1}{12}\kappa F_{1,x_1x_1x_1x_1} - \tfrac{3}{32}\Gamma^2|F_1|^4 F_1.\end{aligned} \tag{3.8}$$

Now we make the substitution $F_3 = F_1 P$ and note that it is sufficient to consider Ω and B of the form $\Omega = \omega_4 t_4$ and $B = \beta x_3$

$$\begin{aligned}0 = P_{x_1x_1} - P_{x_1}\Gamma A\tanh\left(\frac{1}{2}\Gamma A x_1\right) + \frac{1}{4}\Gamma^2 A^2 P\left[1 - 2\,\mathrm{sech}^2\left(\frac{1}{2}\Gamma A x_1\right)\right]\\ + \frac{1}{2}\Gamma^2 A^2\,\mathrm{sech}^2\left(\frac{1}{2}\Gamma A x_1\right)(2P + \bar{P}) - 2\mathrm{i}\Gamma P_{t_2} - \frac{1}{4}\Gamma^2 A^2 P\\ + \frac{1}{192}\kappa\Gamma^4 A^4\left[1 - 20\,\mathrm{sech}^2\left(\frac{1}{2}\Gamma A x_1\right) + 24\,\mathrm{sech}^4\left(\frac{1}{2}\Gamma A x_1\right)\right]\\ - \frac{3}{32}\Gamma^2 A^4\,\mathrm{sech}^4\left(\frac{1}{2}\Gamma A x_1\right) + \Gamma A\frac{\partial B}{\partial x_3}\left[1 - 2\,\mathrm{sech}^2\left(\frac{1}{2}\Gamma A x_1\right)\right]\\ + \frac{1}{64}\Gamma^2 A^4 + 2\Gamma\frac{\partial\Omega}{\partial t_4}.\end{aligned} \tag{3.9}$$

Due to the special form of this equation, the solution $P(x_1, t_2)$ can be expressed in terms of a power series in $\mathrm{sech}^2\left(\frac{1}{2}\Gamma A x_1\right)$, with coefficients dependent on t_2, namely $P(x_1, t_2) = \sum_n a_n(t_2)\mathrm{sech}^{2n}\left(\frac{1}{2}\Gamma A x_1\right)$. This simplification requires the two unknown derivatives $\partial B/\partial x_3$ and $\partial\Omega/\partial t_4$ to be constant, hence we define $\beta = \partial B/\partial x_3$ and $\omega_4 = \partial\Omega/\partial t_4$. Further analysis reveals that a finite sum—in fact just the first two terms—is sufficient to solve the partial differential equation exactly. Hence $P = a_0(t_2) + a_1(t_2)\,\mathrm{sech}^2(\frac{1}{2}\Gamma A x_1)$ for suitable functions

$a_0(t_2)$, $a_1(t_2)$ which are yet to be determined. When this is substituted into the above and the coefficients of powers of $\mathrm{sech}^2(\frac{1}{2}\Gamma A x_1)$ are equated, the resulting system of algebraic and ordinary differential equations is

$$\begin{aligned} 0 &= -2a_1(t_2) + \frac{1}{2}\bar{a}_1(t_2) - \frac{3}{32}A^2 + \frac{1}{8}\kappa\Gamma^2A^2 \\ 0 &= 2a_1(t_2) - \frac{2\mathrm{i}}{\Gamma A^2}\frac{\mathrm{d}a_1}{\mathrm{d}t_2} + \frac{1}{2}a_0(t_2) + \frac{1}{2}\bar{a}_0(t_2) - \frac{2\beta}{\Gamma A} - \frac{5}{48}\kappa\Gamma^2A^2 \\ \frac{2\mathrm{i}}{\Gamma A^2}\frac{\mathrm{d}a_0}{\mathrm{d}t_2} &= \frac{\beta}{\Gamma A} + \frac{1}{64}A^2 + \frac{1}{192}\kappa\Gamma^2A^2 + \frac{2\omega_4}{\Gamma A^2}. \end{aligned} \tag{3.10}$$

The secularity condition required by the multiple scales analysis is $\partial P/\partial t_2 = 0$ which implies that $a_0'(t_2) = 0$ and $a_1'(t_2) = 0$. This ensures that F_3 will be periodic in t_2 and not subject to any resonant interactions with earlier terms in the asymptotic expansion. Thus a_0, a_1 are constants and not dependent on t_2. Hence we now have four constants to find: a_0, a_1, β and ω_4, and so one requires a further equation as (3.10) gives only three conditions. The final condition comes from our definition of ε described earlier. This states that $\phi(0,0) = 2\varepsilon A$ exactly, so the sum of the two $\mathcal{O}(\varepsilon^3)$ terms cannot alter the amplitude of the breather. Thus $F_3(0, 0 + G_3(0,0) = 0$ and since G_3 is already known

$$a_0 + a_1 = P|_{x=0} = \frac{F_3(0,0,0,0)}{F_1(0,0,0,0)} = \frac{-G_3(0,0,0,0)}{F_1(0,0,0,0)} = \frac{1}{48}A^2. \tag{3.11}$$

This, together with (3.10), determines all four unknown constants, a_0, a_1, ω_4 and β

$$\begin{aligned} &\beta = -\tfrac{1}{48}\Gamma A^3(1 + \tfrac{1}{2}\kappa\Gamma^2) \qquad a_0 = \tfrac{1}{12}A^2(1 - \kappa\Gamma^2) \\ &\omega_4 = \tfrac{1}{384}\Gamma A^4(1 + \kappa\Gamma^2) \qquad a_1 = -\tfrac{1}{16}A^2(1 - \tfrac{4}{3}\kappa\Gamma^2). \end{aligned} \tag{3.12}$$

Putting $\mu = \varepsilon A/2$, gives the shape at $t = 0$

$$\phi_n \sim 4\mu\,\mathrm{sech}(\varrho n)[1 + \tfrac{1}{3}\mu^2(1 - \kappa\Gamma^2)\tanh^2(\varrho n)]. \tag{3.13}$$

This agrees with the expansion of the known pure SG breather in the case $\kappa = 0$ and when $\kappa = 1$, gives the corrections caused by the discrete nature of the DSG system. Also we can obtain the time-dependent solution

$$\begin{aligned} &\omega \sim \Gamma[1 - \tfrac{1}{2}\mu^2 + \tfrac{1}{24}\mu^4(1 - \kappa\Gamma^2)] \sim \Gamma\cos\mu - \tfrac{1}{24}\kappa\Gamma^3\mu^4 \\ &\varrho \sim \Gamma[\mu - \tfrac{1}{6}\mu^3(1 - \tfrac{1}{2}\kappa\Gamma^2)] \sim \Gamma\sin\mu + \tfrac{1}{12}\kappa\Gamma^3\mu^3 \\ &\phi_n \sim 4\mu\cos(\omega t)\,\mathrm{sech}(\varrho n)[1 + \tfrac{1}{3}\mu^2\{1 - \cos^2(\omega t)\,\mathrm{sech}^2(\varrho n) - \kappa\Gamma^2\tanh^2(\varrho n)\}] \end{aligned} \tag{3.14}$$

which, in the case $\kappa = 0$, agrees with the direct expansion of the known SG breather.

This calculation also shows that discreteness affects the shape of the breather at a lower order of breather amplitude than it affects the frequency. The frequency corrections are $\mathcal{O}(\Gamma^3\mu^4)$ whereas shape corrections are $\mathcal{O}(\Gamma^3\mu^3)$. This observation has been made for this system by use of other approximation methods [13]. A major improvement in the current results is that we not only predict narrower breathers in a discrete system, as in earlier work, but we now also find the full shape modification in the small amplitude limit.

3.2. Solution of the (2,2) Padé equation

In this section we solve equation (2.3) using a series expansion of the same form as (3.3). *A priori* we treat the functions F_1, F_3, G_3, etc as unknowns, possibly different to those found in the above section. Ultimately, we will find the same solutions for them as above; however, intermediate stages of the calculation differ.

The asymptotic expansion is substituted into the small amplitude expansion of (2.3), namely

$$\phi_{tt} = -\Gamma^2\phi + \tfrac{1}{6}\Gamma^2\phi^3 - \tfrac{1}{120}\Gamma^2\phi^5 + \phi_{xx} + \tfrac{1}{12}\phi_{xxtt} + \tfrac{1}{12}\Gamma^2\phi_{xx} - \tfrac{1}{12}\Gamma^2\phi_x^2\phi - \tfrac{1}{24}\Gamma^2\phi^2\phi_{xx} \tag{3.15}$$

to give another hierarchy of equations in orders of ε and harmonics of the fundamental frequency Γ.

Since we do not require F_5, there is no need to find the other $\mathcal{O}(\varepsilon^5)$ correction terms, G_5 and H_5. Thus we shall not quote their determining equations—those obtained by considering terms of orders $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$ and $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{5\mathrm{i}\Gamma t_0})$.

Separating out the different frequencies ($\mathrm{e}^{\mathrm{i}\Gamma t_0}$, $\mathrm{e}^{3\mathrm{i}\Gamma t_0}$) and different orders of ε produces the following

$\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$2\mathrm{i}\Gamma F_{1,t_2} = F_{1,x_1x_1} + \tfrac{1}{2}\Gamma^2|F_1|^2F_1$$

$\mathcal{O}(\varepsilon^3\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$:

$$-9\Gamma^2G_3 = -\Gamma^2G_3 + \tfrac{1}{6}\Gamma^2F_1^3$$

$\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$\begin{aligned}2\mathrm{i}\Gamma F_{3,t_2} + 2\mathrm{i}\Gamma F_{1,t_4} + F_{1,t_2t_2} = {} & F_{3,x_1x_1} + 2F_{1,x_1x_3} + \tfrac{1}{2}\Gamma^2F_1^2\bar{F}_3 + \Gamma^2|F_1|^2F_3 + \tfrac{1}{2}\Gamma^2\bar{F}_1^2G_3 \\ & -\tfrac{1}{12}\Gamma^2|F_1|^4F_1 - \tfrac{1}{12}\Gamma^2F_{3,x_1x_1} - \tfrac{1}{6}\Gamma^2F_{1,x_1x_3} + \tfrac{1}{6}\mathrm{i}\Gamma F_{1,x_1x_1t_2} + \tfrac{1}{12}\Gamma^2F_{3,x_1x_1} \\ & +\tfrac{1}{6}\Gamma^2F_{1,x_1x_3} - \tfrac{1}{12}\Gamma^2|F_1|^2F_{1,x_1x_1} - \tfrac{1}{24}\Gamma^2F_1^2\bar{F}_{x_1x_1} - \tfrac{1}{6}\Gamma^2|F_{1,x_1}|^2F_1 \\ & -\tfrac{1}{12}\Gamma^2F_{1,x_1}^2\bar{F}_1.\end{aligned} \tag{3.16}$$

The $\mathcal{O}(\varepsilon\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ equation is trivially satisfied. The $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ equation is the same NLS equation as was derived in the (4,0) Padé approximation, and so has the same solution (3.6) as given there. Again the $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ equation gives the higher frequency correction

$$G_3 = -\tfrac{1}{48}F_1^3 = -\tfrac{1}{48}A^3\,\mathrm{e}^{3\mathrm{i}\Omega-3\mathrm{i}\Gamma A^2t_2/8}\,\mathrm{sech}^3(\tfrac{1}{2}\Gamma Ax_1 + B). \tag{3.17}$$

We shall solve the $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ equation to find F_3, the $\mathcal{O}(\varepsilon^3)$ correction to the breather. This equation has marked differences to the $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ equation from the previous calculation (3.5). For example, we no longer have a $F_{1,x_1x_1x_1x_1}$ term but do have a $F_{1,x_1x_1t_2}$ term as well as several others not present in (3.5). Fortunately, however, the last equation of (3.16) is still amenable to solution using the same methods. We write $F_3 = F_1P$ where $P = P(x_1, t_2)$ is subject to the secularity condition $\partial P/\partial t_2 = 0$; hence, we shall treat P as a function purely of x_1 and obtain an ordinary differential equation for $P(x_1)$

$$\begin{aligned}\frac{2\mathrm{i}\Gamma PF_{1,t_2}}{F_1} = {} & P_{x_1x_1} + \frac{2P_{x_1}F_{1,x_1}}{F_1} + \frac{PF_{1,x_1x_1}}{F_1} - \frac{2\mathrm{i}\Gamma F_{1,t_4}}{F_1} - \frac{F_{1,t_2t_2}}{F_1} + \frac{2F_{1,x_1x_3}}{F_1} \\ & +\frac{1}{2}\Gamma^2|F_1|^2\bar{P} + \Gamma^2|F_1|^2P - \frac{3\Gamma^2|F_1|^4}{32} + \frac{\mathrm{i}\Gamma F_{1,x_1x_1t_2}}{6F_1} - \frac{\Gamma^2\bar{F}_1F_{1,x_1x_1}}{12} \\ & -\frac{\Gamma^2F_1\bar{F}_{1,x_1x_1}}{24} - \frac{\Gamma^2F_{1,x_1}}{12F_1}(\bar{F}_1F_{1,x_1} + 2F_1\bar{F}_{1,x_1}).\end{aligned} \tag{3.18}$$

As above, a solution of this can be found in terms of a finite power series of $\mathrm{sech}^2(\tfrac{1}{2}\Gamma Ax_1)$; substituting $P(x_1) = a_0 + a_1\mathrm{sech}^2(\tfrac{1}{2}\Gamma Ax_1)$ leads to equations for a_0, a_1, ω_4 and $\beta = \partial B/\partial x_3$, by equating the coefficients of powers of $\mathrm{sech}^2(\tfrac{1}{2}\Gamma Ax_1)$. The final equation needed for a fully determined system comes from the boundary condition

$P(0) = \frac{1}{48}A^2$, since by our definition of ε, the $\mathcal{O}(\varepsilon^3)$ terms must make no alteration to the amplitude of the breather:

$$\begin{aligned} 0 &= \frac{8\omega_4}{\Gamma A^2} + \frac{A^2}{16} + \frac{4\beta}{\Gamma A} + \frac{\Gamma^2 A^2}{48} \\ 0 &= 8a_1 + 2a_0 - \frac{8\beta}{\Gamma A} + 2\bar{a}_0 - \frac{5}{12}\Gamma^2 A^2 \\ 0 &= -8a_1 + 2\bar{a}_1 - \frac{3}{8}A^2 + \frac{1}{2}\Gamma^2 A^2 \\ \frac{1}{48}A^2 &= a_0 + a_1. \end{aligned} \tag{3.19}$$

The solution of this system is identical to the $\kappa = 1$ case of (3.12). Hence the shape at $t = 0$ and the full temporal evolution is identical to that for the (4,0) Padé approximation.

3.3. Solution of the (4,2) Padé equation

Finally in this section, for the sake of completeness, we outline a similar calculation for the complex, but also more accurate (4,2) Padé approximation of the DSG system. The small amplitude expansion of (2.6) which we aim to solve is

$$\begin{aligned} \phi_{tt} = {} & -\Gamma^2\phi + \tfrac{1}{6}\Gamma^2\phi^3 - \tfrac{1}{120}\Gamma^2\phi^5 + \phi_{xx} + \tfrac{1}{30}\phi_{xxtt} + \tfrac{1}{20}\phi_{xxxx} + \tfrac{1}{30}\Gamma^2\phi_{xx} \\ & - \tfrac{1}{60}\Gamma^2\phi^2\phi_{xx} - \tfrac{1}{30}\Gamma^2\phi_x^2\phi. \end{aligned} \tag{3.20}$$

The asymptotic ansatz (3.3) is once again assumed and inserted, and equating coefficients of powers of ε and harmonics of $e^{i\Gamma t_0}$ yields a hierarchy of equations. The $\mathcal{O}(\varepsilon^3 e^{i\Gamma t_0})$ terms give the NLS equation exactly as in the previous two approximations, and the $\mathcal{O}(\varepsilon^3 e^{3i\Gamma t_0})$ terms also yield the same equation as before (3.17).

Thus the solutions for F_1 and G_3 are also the same as before with F_1 being given by (3.6) and G_3 by (3.17). Terms of $\mathcal{O}(\varepsilon^5 e^{i\Gamma t_0})$ generate a new equation for F_3

$$\begin{aligned} 2i\Gamma F_{1,t_4} + F_{1,t_2t_2} + 2i\Gamma F_{3,t_2} = {} & \tfrac{1}{2}\Gamma^2(F_1^2\bar{F}_3 + G_3\bar{F}_1^2 + 2|F_1|^2F_3) \\ & - \tfrac{1}{12}\Gamma^2|F_1|^4F_1 + F_{3,x_1x_1} + 2F_{1,x_1x_3} + \tfrac{1}{20}F_{1,x_1x_1x_1x_1} + \tfrac{1}{30}\Gamma^2F_{3,x_1x_1} \\ & + \tfrac{1}{15}\Gamma^2F_{1,x_1x_3} - \tfrac{1}{60}\Gamma^2(F_1^2\bar{F}_{1,x_1x_1} + 2F_{1,x_1x_1}|F_1|^2) + \tfrac{1}{15}i\Gamma F_{1,x_1x_1t_2} \\ & - \tfrac{1}{30}\Gamma^2(\bar{F}_1F_{1,x_1}^2 + 2F_1|F_{1,x_1}|^2) - \tfrac{1}{30}\Gamma^2F_{3,x_1x_1} - \tfrac{1}{15}\Gamma^2F_{1,x_1x_3}. \end{aligned} \tag{3.21}$$

Writing $\theta = \frac{1}{2}\Gamma A x_1 + B$, and $F_3 = F_1 P$ (as before) we find

$$\begin{aligned} -\frac{2\omega_4}{\Gamma} - \frac{A^4}{64} + \frac{A^2P}{4} + \frac{2iP_{t_2}}{\Gamma} = {} & \frac{3}{2}A^2P\,\mathrm{sech}^2\theta - \frac{3}{32}A^4\,\mathrm{sech}^4\theta \\ & + \frac{1}{4}A^2P(1-\mathrm{sech}^2\theta) - \frac{AP_{x_1}}{\Gamma}\tanh\theta + \frac{P_{x_1x_1}}{\Gamma^2} + \frac{A}{\Gamma^2}\frac{dB}{dx_3}(1-2\,\mathrm{sech}^2\theta) \\ & + \frac{1}{320}\Gamma^2A^4(1-20\,\mathrm{sech}^2\theta + 24\,\mathrm{sech}^4\theta) + \frac{1}{480}\Gamma^2A^4(1-2\,\mathrm{sech}^2\theta) \\ & - \frac{1}{80}\Gamma^2A^4(3-4\,\mathrm{sech}^2\theta)\,\mathrm{sech}^2\theta. \end{aligned} \tag{3.22}$$

This has the same solution as in the previous two calculations. The solution for P is $a_0(t_2) + a_1(t_2)\,\mathrm{sech}^2\theta$ and the secularity conditions are $a_0' = 0 = a_1'$ giving a system of three equations. The final condition is once again due to the definition of ε which implies that the $\mathcal{O}(\varepsilon^3)$ terms make no contribution to the amplitude of the breather. Thus the final solution for F_3 is the same as determined from the earlier approximations, and is given by the above substitutions with a_0, a_1, β and ω_4 as specified in (3.12) with $\kappa = 1$.

This shows that the three approximating PDEs (2.1), (2.3) and (2.6) all generate the same breather solution. From this we may deduce that the approximation technique leaves invariant the underlying nonlinear dynamics of the DSG equation at least in the long wavelength limit. It has been shown earlier that some of them are more faithful in their reproduction of the linear dynamics of the discrete system than others.

4. PDE approximations to the generalized Klein–Gordon lattice

In this section we shall analyse the generalized Klein–Gordon equation (1.10) which was derived in the introduction. First let us perform a minor rescaling of (1.10) and denote the Taylor series of the nonlinear interaction by

$$2V'(\phi) + 4h\phi = \tilde{V}'(\phi) = \Gamma^2\phi(1 - \gamma_1\phi - \gamma_2\phi^2 - \gamma_3\phi^3 - \gamma_4\phi^4). \qquad (4.1)$$

Thus the small-amplitude expansion of equation we aim to solve is

$$\begin{aligned}\ddot{\phi}_n = {} & (f - h)(\phi_{n+1} - 2\phi_n + \phi_{n-1}) + g(\phi_{n+2} - 2\phi_n + \phi_{n-2}) \\ & -\Gamma^2\phi_n(1 - \gamma_1\phi_n - \gamma_2\phi_n^2 - \gamma_3\phi_n^3 - \gamma_4\phi_n^4). \end{aligned} \qquad (4.2)$$

The odd symmetry ($\phi \mapsto -\phi$) present in the DSG equation is destroyed by the γ_1, γ_3 terms. This equation is also a generalization of the usual nonlinear discrete Klein–Gordon equation due to the presence of second-neighbour interactions.

A family of partial differential equations which approximate this can be constructed using the methods outlined in section 2, namely that of rewriting the system of ordinary differential equations as an operator equation acting on functions of two continuous variables. We then approximate the spatial difference operator in terms of a ratio of polynomials in the differential operator; this yields a simpler equation whose solution approximates the solution of the original (discrete) system. All of the approximations we propose initially require the spatial differences to be expanded in a Taylor series

$$\begin{aligned}\phi_{tt} = {} & -\tilde{V}'(\phi) + [(f - h)(\mathrm{e}^{\partial_x} - 2 + \mathrm{e}^{-\partial_x}) + g(\mathrm{e}^{2\partial_x} - 2 + \mathrm{e}^{-2\partial_x})]\phi \\ = {} & -\tilde{V}'(\phi) + (f - h + 4g)\left[\partial_x^2 + \frac{(f - h + 16g)}{12(f - h + 4g)}\partial_x^4 + \frac{(f - h + 64g)}{360(f - h + 4g)}\partial_x^6\right] \\ & \times\phi + \mathcal{O}(\partial_x^8\phi). \end{aligned} \qquad (4.3)$$

The various PDEs are generated by using different approximations to the operator in square brackets. The four simplest approximations are described in the following, together with a brief description of the behaviour of linear modes to establish which are well-posed.

4.1. (2,0) Padé approximation

In our notation, the (2,0) Padé approximate corresponds to the standard continuum approximation where the discrete second central difference operator is simply replaced by a second derivative. The resulting partial differential equation is a continuous Klein–Gordon equation

$$\phi_{tt} = (f - h + 4g)\phi_{xx} - \Gamma^2\phi(1 - \gamma_1\phi - \gamma_2\phi^2 - \gamma_3\phi^3 - \gamma_4\phi^4). \qquad (4.4)$$

Equations of this form have been widely studied, but can oversimplify the dynamics of the discrete equation. In the specific case of DSG, the standard continuum approximation leads to the SG equation—an integrable equation with many properties not shared by the DSG equation. As another illustration of this we compare the dispersion relation of (4.4)

$$\omega^2 = \Gamma^2 + (f - h + 4g)k^2 \tag{4.5}$$

with that for the fully discrete model (1.12). The dispersion relation for the full model occupies a finite band of frequencies, where as this approximation allows $\omega \to \infty$ for large wavenumbers.

4.2. (4,0) Padé approximation

A simple truncation of the operator expansion (4.3) at fourth order leads to the (4,0) Padé approximate

$$\phi_{tt} = (f - h + 4g)\phi_{xx} - \tilde{V}'(\phi) + \tfrac{1}{12}(f - h + 16g)\phi_{xxxx} \tag{4.6}$$

which is the simplest of the more accurate quasi-continuum approximations. This, however, has the property that for large wavenumbers its dispersion relation

$$\omega^2 = \Gamma^2 + (f - h + 4g)k^2 - \tfrac{1}{12}(f - h + 16g)k^4 \tag{4.7}$$

diverges, and if $f - h + 16g > 0$, the frequency ω becomes complex implying that the zero solution of this equation is unstable to high wavenumbers—a property that the discrete system does not possess in the same parameter range. The extra accuracy that this higher-order approximation achieves is reflected in that its dispersion relation is closer to (1.12) for small wavenumbers.

This is the only one of the more accurate approximations which maintains the Lagrangian and Hamiltonian structure of the original system (1.8). Equation (4.6) can be generated from the Lagrangian density $\mathcal{L} = \frac{1}{2}\phi_t^2 - \frac{1}{2}(f - h + 4g)\phi_x^2 - \tilde{V}(\phi) + \frac{1}{24}(f - h + 16g)\phi_{xx}^2$.

4.3. (2,2) Padé approximation

An alternative equation can be generated by using the (2,2) Padé approximation to the term in square brackets in (4.3)

$$\phi_{tt} = (f - h + 4g)\phi_{xx} - \tilde{V}'(\phi) + \frac{(f - h + 16g)}{12(f - h + 4g)}(\phi_{xxtt} + \tilde{V}''(\phi)\phi_{xx} + \tilde{V}'''(\phi)\phi_x^2). \tag{4.8}$$

This formally has the same order of accuracy as the (4,0) Padé approximation (4.6), and has the dispersion relation

$$\omega^2 = \frac{(f - h + 4g)\Gamma^2 + (f - h + 4g)^2k^2 + \frac{1}{12}\Gamma^2k^2(f - h + 16g)}{(f - h + 4g) + \frac{1}{12}k^2(f - h + 16g)}. \tag{4.9}$$

Provided $(f - h + 4g)^2/(f - h + 16g) > -\frac{1}{12}\Gamma^2$, the frequency ω occupies only a finite band of frequencies between Γ and $\sqrt{[\Gamma^2 + 12(f - h + 4g)^2/(f - h + 16g)]}$. This property is qualitatively the same as the full dispersion relation (1.12). If $(f - h + 16g)(f - h + 4g) < 0$ then the denominator vanishes for some wavenumber k_c and the dispersion relation predicts unstable waves for $k \gtrapprox k_c$.

4.4. (4,2) Padé approximation

The final approximation we shall consider is formally more accurate than any of the above. The last two only consider terms up to $\mathcal{O}(\partial_x^4)$ of the expansion of the original operator equation (4.3), whereas we shall now include the $\mathcal{O}(\partial_x^6)$ term as well. The (4,2) Padé approximate is

$$\phi_{tt} = (f-h+4g)\phi_{xx} - \tilde{V}'(\phi) + \left(\frac{(f-h)^2 + 8g(f-h) + 256g^2}{20(f-h+16g)}\right)\phi_{xxxx} + \frac{(f-h+64g)}{30(f-h+16g)}(\phi_{xxtt} + \tilde{V}''(\phi)\phi_{xx} + \tilde{V}'''(\phi)\phi_x^2). \tag{4.10}$$

This approximation also has a dispersion relation which diverges for large k, but only in the manner of $\mathcal{O}(k^2)$ and, not as strongly as the (4,0) Padé approximation which diverges like $\mathcal{O}(k^4)$. The dispersion relation for the (4,2) Padé approximation is

$$\omega^2 = \{(f-h+16g)[\Gamma^2 + k^2(f-h+4g)] + \tfrac{1}{30}\Gamma^2 k^2(f-h+64g) - \tfrac{1}{20}k^4[(f-h)^2 + 8g(f-h) + 256g^2]\}\{(f-h+16g) + \tfrac{1}{30}k^2(f-h+64g)\}^{-1}. \tag{4.11}$$

This does not have a finite band of allowable linear frequencies which the system of ordinary differential equations possesses (1.12). Depending on Γ and g, this approximation to ω^2 can remain positive everywhere—demonstrating that there is a suitable well-posed PDE approximation to the system of ordinary differential equations (4.2).

4.5. Summary of results

The (4,2) Padé and (2,2) Padé equations are very similar in a number terms: apart from differences in coefficients, the only difference is the presence of a ϕ_{xxxx} term in the (4,2) approximate. The set of terms $\phi_{xxtt} + \tilde{V}''(\phi)\phi_{xx} - \tilde{V}'''(\phi)\phi_x^2$ derived in the (2,2) Padé approximation introduces extra nonlinearities to the PDE approximation. It is an alternative correction term to the more common ϕ_{xxxx} seen in the (4,0) approximate. The (4,2) approximation combines the two correction terms to form a yet more accurate approximating equation.

Figure 3 shows the dispersion relation for the lattice with $f-h=1$, $g=-0.05$ and $\Gamma=0.236$, and the dispersion relation for each of the partial differential equation approximations derived. All are asymptotic to the exact solution in the limit $k \to 0$, but have wildly differing behaviours for k away from zero.

With the parameters used in the figure, the (4,2) Padé approximation contains singularities at $k = \pm\sqrt{(30/11)} \approx \pm 1.65$. The (4,0) Padé approximate predicts the frequency increasing for as k increases to 5 then decreasing again, vanishing at $k \approx 7$. The PDE is unstable to wavenumbers above this limit. The standard continuum approximation does not suffer from such a problem, rather it predicts arbitrarily large frequencies for large wavenumbers, which is again not a property of the lattice. The best qualitative approximation to the dispersion relation comes from the (2,2) Padé method, whose frequencies all lie in the range $0.236 \leqslant \omega \leqslant 6.20$, whereas the lattice's linear frequencies all lie in the band $0.236 \leqslant \omega \leqslant 2.01$.

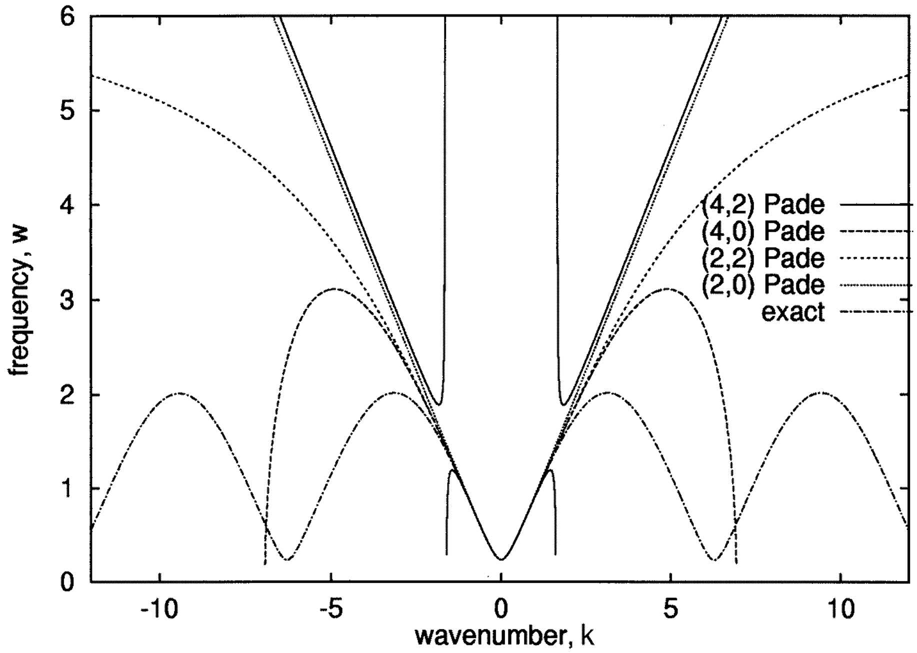

Figure 3. Dispersion relations for the generalized discrete nonlinear Klein–Gordon equation and PDE approximations to it (with $\Gamma = 0.236$ and $g = -0.05$).

5. Breather solution of the generalized lattice

We now aim to use one of the more accurate PDEs—namely the (4,0) Padé approximate—to find a highly accurate asymptotic approximation to the breather mode of the generalized discrete nonlinear Klein–Gordon lattice (4.2). When trying to find moving breathers in a Klein–Gordon equation with quadratic nonlinearity, Peyrard and Bishop [9] used a NLS-type reduction

$$\phi_n = F_1(\varepsilon n, \varepsilon t)\, e^{i(kn-\omega(k)t)} + \varepsilon[G_2(\varepsilon n, \varepsilon t) + H_2(\varepsilon n, \varepsilon t)\, e^{2i(kn-\omega(k)t)}] + \text{CC} \tag{5.1}$$

where $\omega(k)$ satisfies the dispersion relation. The non-oscillatory and second-harmonic terms on the $\mathcal{O}(1)$ timescale, G_2 and H_2, are necessary to balance the even powers of ϕ that occur in the power series expansion of the nonlinear potential.

We shall use a generalization of (5.1) to find the corrections to a stationary breather caused by the discrete nature of the underlying spatial dimension. The long time scales t_2, t_4 and space scales x_1, x_3 are identical to those used in the DSG equation (3.1). Our higher-order approximation must now include even powers of the fundamental frequency ($e^{i\Gamma t_0}$) at even orders of the small parameter ε. Thus we postulate that the solution has the form of an asymptotic series which is considerably more general than that used previously. In place of (3.3), we use the ansatz

$$\begin{aligned}\phi = \varepsilon\, e^{i\Gamma t_0} F_1 + \varepsilon^2(G_2 + e^{2i\Gamma t_0} H_2) + \varepsilon^3(e^{i\Gamma t_0} F_3 + e^{3i\Gamma t_0} J_3) + \varepsilon^4(G_4 + e^{2i\Gamma t_0} H_4 + e^{4i\Gamma t_0} K_4) \\ + \varepsilon^5(e^{i\Gamma t_0} F_5 + e^{3i\Gamma t_0} J_5 + e^{5i\Gamma t_0} L_5) + \text{CC}\end{aligned} \tag{5.2}$$

to determine the changes in shape that are caused by the discrete structure underlying our generalized nonlinear Klein–Gordon lattice. Here, all the quantities F_1, G_2, H_2, F_3, J_3, G_4,

H_4, K_4, F_5, J_5 and L_5 are functions of (x_1, t_2, x_3, t_4), although it will not be necessary for us to find expressions for all of them.

We shall use the notation $\Delta_2 = f - h + 4g$, $\Delta_4 = \frac{1}{12}(f - h + 16g)$, in order to write the equation we aim to solve as

$$\phi_{tt} = \Delta_2\phi_{xx} + \Delta_4\phi_{xxxx} - \Gamma^2\phi(1 - \gamma_1\phi - \gamma_2\phi^2 - \gamma_3\phi^3 - \gamma_4\phi^4). \tag{5.3}$$

Substituting (5.2) into (5.3) and equating terms of the same order in ε and of the same harmonic (power of $\mathrm{e}^{\mathrm{i}\Gamma t_0}$) leads to the hierarchy of equations

$\mathcal{O}(\varepsilon^2\,\mathrm{e}^{0\mathrm{i}\Gamma t_0})$:

$$0 = -\Gamma^2 G_2 + \Gamma^2\gamma_1|F_1|^2$$

$\mathcal{O}(\varepsilon^2\,\mathrm{e}^{2\mathrm{i}\Gamma t_0})$:

$$-4\Gamma^2 H_2 = -\Gamma^2 H_2 + \Gamma^2\gamma_1 F_1^2$$

$\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$2\mathrm{i}\Gamma F_{1,t_2} = \Delta_2 F_{1,x_1x_1} + 2\gamma_1\Gamma^2[F_1G_2 + \bar{F}_1H_2 + F_1\bar{G}_2] + 3\gamma_2\Gamma^2|F_1|^2F_1$$

$\mathcal{O}(\varepsilon^3\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$:

$$-9\Gamma^2 J_3 = -\Gamma^2 J_3 + 2\gamma_1\Gamma^2F_1H_2 + \gamma_2\Gamma^2F_1^3$$

$\mathcal{O}(\varepsilon^4\,\mathrm{e}^{0\mathrm{i}\Gamma t_0})$:

$$\begin{aligned}0 = \Delta_2(G_{2,x_1x_1} + \bar{G}_{2,x_1x_1}) &- \Gamma^2(G_4 + \bar{G}_4) + 6\gamma_3\Gamma^2|F_1|^4\\ &+\gamma_1\Gamma^2[2F_1\bar{F}_3 + 2\bar{F}_1F_3 + (G_2 + \bar{G}_2)^2 + 2|H_2|^2]\\ &+3\gamma_2\Gamma^2[F_1^2\bar{H}_2 + \bar{F}_1^2H_2 + 2|F_1|^2(G_2 + \bar{G}_2)]\end{aligned}$$

$\mathcal{O}(\varepsilon^4\,\mathrm{e}^{2\mathrm{i}\Gamma t_0})$:

$$\begin{aligned}-4\Gamma^2H_4 + 4\mathrm{i}\Gamma H_{2,t_2} = \Delta_2 H_{2,x_1x_1} &- \Gamma^2H_4 + 4\gamma_3\Gamma^2|F_1|^2F_1^2\\ &+3\gamma_2\Gamma^2[F_1^2G_2 + F_1^2\bar{G}_2 + 2|F_1|^2H_2]\\ &+\gamma_1\Gamma^2[2F_1F_3 + 2\bar{F}_1J_3 + 2G_2H_2 + 2\bar{G}_2H_2]\end{aligned}$$

$\mathcal{O}(\varepsilon^4\,\mathrm{e}^{4\mathrm{i}\Gamma t_0})$:

$$-16\Gamma^2K_4 = -\Gamma^2K_4 + \gamma_1\Gamma^2H_2^2 + 2\gamma_1\Gamma^2F_1J_3 + \gamma_3\Gamma^2F_1^4 + 3\gamma_2\Gamma^2F_1^2H_2$$

$\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$:

$$\begin{aligned}2\mathrm{i}\Gamma F_{3,t_2} + F_{1,t_2t_2} + 2\mathrm{i}\Gamma F_{1,t_4} = \Delta_2F_{3,x_1,x_1} &+ 2\Delta_2F_{1,x_1x_3} + \Delta_4F_{1,x_1x_1x_1x_1} + 10\gamma_4\Gamma^2|F_1|^4F_1\\ &+4\gamma_3\Gamma^2[F_1^3\bar{H}_2 + 3|F_1|^2F_1(G_2 + \bar{G}_2) + 3|F_1|^2\bar{F}_1H_2]\\ &+3\gamma_2\Gamma^2[F_1(G_2 + \bar{G}_2)^2 + 2\bar{F}_1H_2(G_2 + \bar{G}_2)\\ &+2|H_2|^2F_1 + \bar{F}_1^2J_3 + F_1^2\bar{F}_3 + 2|F_1|^2F_3]\\ &+2\gamma_1\Gamma^2[F_1(G_4 + \bar{G}_4) + \bar{F}_1H_4 + \bar{F}_3H_2 + F_3(G_2 + \bar{G}_2) + \bar{H}_2J_3].\end{aligned} \tag{5.4}$$

In such a reduction, the $\mathcal{O}(\varepsilon\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ term is trivially satisfied; the two $\mathcal{O}(\varepsilon^2)$ terms and $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{3\mathrm{i}\Gamma t_0})$ term imply

$$G_2 = \gamma_1|F_1|^2 \qquad H_2 = -\tfrac{1}{3}\gamma_1F_1^2 \qquad J_3 = \tfrac{1}{24}(2\gamma_1^2 - 3\gamma_2)F_1^3. \tag{5.5}$$

However, the $\mathcal{O}(\varepsilon^3\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ term is not so simple: this now reduces to

$$2\mathrm{i}\Gamma F_{1,t_2} = \Delta_2F_{1,x_1x_1} + \tfrac{1}{3}\Gamma^2(10\gamma_1^2 + 9\gamma_2)|F_1|^2F_1. \tag{5.6}$$

In the DSG expansion we had $\Delta_2 = 1$, $\gamma_1 = 0$, $\gamma_2 = \frac{1}{6}$, so that both the terms on the right-hand side had positive coefficients. Now we wish to consider the additional possibilities of Δ_2 being negative, and/or $\gamma_2 < -\frac{10}{9}\gamma_1^2$. There are two distinct types of solution: the bright soliton, which we have already encountered, occurs when the two coefficients have the same signs. This can be written

$$F_1 = A\,\mathrm{e}^{\mathrm{i}\Omega}\,\mathrm{e}^{-\mathrm{i}\Gamma A^2(10\gamma_1^2+9\gamma_2)t_2/12}\,\mathrm{sech}\left(\Gamma A x_1\sqrt{\frac{10\gamma_1^2+9\gamma_2}{6\Delta_2}} + B\right). \tag{5.7}$$

The new phenomenon occurs when the sign of the nonlinearity is opposite to that of the dispersive term: then the dark (or 'hole') soliton solution occurs. In its simplest form this solution is

$$F_1 = A\,\mathrm{e}^{-\mathrm{i}A^2 t_2/2\Delta_2\Gamma}\tanh\left(\Gamma A x_1 \frac{-(10\gamma_1^2+9\gamma_2)}{6\Delta_2}\right). \tag{5.8}$$

A more general solution is given in Remoissenet [8]. This solution does not induce breather-type solutions in the lattice equation (4.2); hence we shall concentrate on the bright soliton for the remainder of our calculations.

Once F_1 has been found, G_2, H_2 and J_3 are fully determined by (5.5). We proceed to find F_3, G_4, H_4 and K_4 by simplifying the algebra with the substitution $F_3 = F_1 P$. The $\mathcal{O}(\varepsilon^4)$ terms from (5.4) imply

$$\begin{aligned}
G_4 &= \frac{\Delta_2\gamma_1}{\Gamma^2}(|F_1|^2)_{x_1x_1} + \gamma_1(P+\bar{P})|F_1|^2 + \left(3\gamma_3 + 5\gamma_1\gamma_2 + \frac{19}{9}\gamma_1^3\right)|F_1|^4\\
H_4 &= \frac{2\Delta_2\gamma_1}{9\Gamma^2}(F_{1,x_1}^2 - F_1F_{1,x_1x_1}) - \frac{2}{3}\gamma_1F_1^2P - \left(\frac{4}{3}\gamma_3 + \frac{31}{12}\gamma_1\gamma_2 + \frac{59}{54}\gamma_1^3\right)|F_1|^2F_1^2\\
K_4 &= \left(\frac{1}{12}\gamma_1\gamma_2 - \frac{1}{15}\gamma_3 - \frac{1}{54}\gamma_1^3\right)F_1^4.
\end{aligned} \tag{5.9}$$

The equation from the $\mathcal{O}(\varepsilon^5\,\mathrm{e}^{\mathrm{i}\Gamma t_0})$ terms provides an equation for P

$$\begin{aligned}
2\mathrm{i}\Gamma(F_1P)_{t_2} + 2\mathrm{i}\Gamma F_{1,t_4} + F_{1,t_2t_2} &= \Delta_2(F_1P)_{x_1x_1} + 2\Delta_2F_{1,x_1x_3} + \Delta_4F_{1,x_1x_1x_1x_1}\\
&\quad + 10\gamma_4\Gamma^2|F_1|^4F_1 + \tfrac{56}{3}\gamma_3\gamma_1\Gamma^2|F_1|^4F_1 + (\tfrac{107}{12}\gamma_1^2\gamma_2 - \tfrac{3}{8}\gamma_2^2)\Gamma^2|F_1|^4F_1\\
&\quad + 3\gamma_2\Gamma^2|F_1|^2F_1(\bar{P}+2P) + 10\gamma_1^2\Gamma^2|F_1|^2F_1P\\
&\quad + (\tfrac{335}{54}\gamma_1^4 + \tfrac{179}{12}\gamma_1^2\gamma_2 + \tfrac{28}{3}\gamma_3\gamma_1)\Gamma^2|F_1|^4F_1\\
&\quad + \gamma_1^2A^2F_1(10\gamma_1^2+9\gamma_2)(\tfrac{2}{27}\,\mathrm{sech}^4\theta + \tfrac{4}{3}(2\,\mathrm{sech}^2\theta - 3\,\mathrm{sech}^4\theta))
\end{aligned} \tag{5.10}$$

where $\theta = \Gamma A x_1\sqrt{(10\gamma_1^2+9\gamma_2)/6\Delta_2} + \beta x_3$. As in the approximation to breathers in the DSG equation, it is sufficient to seek a solution for P in the form of a finite series in powers of $\mathrm{sech}^2\theta$; in fact just two terms are required: $P = a_0(t_2) + a_2(t_2)\,\mathrm{sech}^2(\theta)$ with $a_0, a_2 \in \mathbb{R}$. The secularity conditions are $\partial P/\partial t_2 = 0$ which implies that $a_0'(t_2) = 0 = a_2'(t_2)$. This leaves four constants to determine: $a_0, a_2, \beta, \omega_4$. Three of the four equations come from equating powers of $\mathrm{sech}^2(\theta)$ in the above equation (5.10). The fourth is generated when we specify that the $\mathcal{O}(\varepsilon^3)$ terms should not generate any extra contribution to the amplitude of the breather (that is at the point $t = 0 = \theta$). This condition reduces to

$$a_0 + a_2 + \tfrac{1}{24}A^2(2\gamma_1^2 - 3\gamma_2) = 0. \tag{5.11}$$

The solution of this system of four equations is

$$a_0 = \frac{-A^2}{18(10\gamma_1^2+9\gamma_2)}\left[\frac{12\Delta_4\Gamma^2(10\gamma_1^2+9\gamma_2)^2}{\Delta_2^2} + 180\gamma_4 - 27\gamma_2^2 - 216\gamma_2\gamma_1^2 + 504\gamma_1\gamma_3 - 580\gamma_1^4\right]$$

$$a_2 = \frac{A^2}{72(10\gamma_1^2+9\gamma_2)}\left[\frac{48\Delta_4\Gamma^2(10\gamma_1^2+9\gamma_2)^2}{\Delta_2^2} + 720\gamma_4 - 27\gamma_2^2 - 828\gamma_2\gamma_1^2 + 2016\gamma_1\gamma_3 - 2380\gamma_1^4\right]$$

$$\beta_3 = \frac{-\Gamma A^3}{36\sqrt{6\Delta_2(10\gamma_1^2+9\gamma_2)}}\left[\frac{6\Delta_4\Gamma^2(10\gamma_1^2+9\gamma_2)^2}{\Delta_2^2} - 1008\gamma_1\gamma_3 - 360\gamma_4 - 220\gamma_1^4 - 27\gamma_2^2 - 900\gamma_2\gamma_1^2\right]$$

$$\omega_4 = \frac{\Gamma A^4}{864}\left[\frac{12\Delta_4\Gamma^2(10\gamma_1^2+9\gamma_2)^2}{\Delta_2^2} - 4032\gamma_1\gamma_3 - 1440\gamma_4 - 351\gamma_2^2 - 4140\gamma_2\gamma_1^2 - 1180\gamma_1^4\right]. \tag{5.12}$$

Knowing the values of these parameters now enables us to write a highly accurate approximation to the breather in closed form. We now quote our results in the original variables x and t using (3.1):

$$\phi = 2\varepsilon A\,\mathrm{sech}(\theta)[\cos(\omega t) + \varepsilon A\gamma_1\{1 - \tfrac{1}{3}\cos(2\omega t)\}\,\mathrm{sech}(\theta) + \varepsilon^2\{(a_0 + a_2\,\mathrm{sech}^2(\theta))\cos(\omega t) + \tfrac{1}{24}A^2(2\gamma_1^2 - 3\gamma_2)\,\mathrm{sech}^2(\theta)\cos(3\omega t)\}] \tag{5.13}$$

where

$$\omega = \Gamma - \frac{1}{12}\Gamma\varepsilon^2A^2(10\gamma_1^2+9\gamma_2) + \varepsilon^4\omega_4 \qquad \theta = \left(\Gamma A\sqrt{\frac{10\gamma_1^2+9\gamma_2}{6\Delta_2}} + \beta\varepsilon^2\right)\varepsilon x. \tag{5.14}$$

It is the terms involving Δ_4 which are introduced as a consequence of treating the discreteness correctly in higher-order terms. The terms influenced are the frequency ω, the space scale θ and more generally the shape of the breather solution through a_0 and a_2. The exact size of these effects depends on the parameters γ_1, γ_2, f, h and g.

As an example of our method, let us apply this approximation to the model of DNA denaturation proposed by Peyrard and Bishop [9]. They assume the nonlinear interaction term has the form of a Morse potential $V(\phi) = D(\mathrm{e}^{-a\phi} - 1)^2$. A Taylor expansion of this leads to the choice of parameters

$$\gamma_1 = \tfrac{3}{2} \qquad \gamma_2 = -\tfrac{7}{6} \qquad \gamma_3 = \tfrac{5}{8} \qquad \gamma_4 = -\tfrac{31}{120} \tag{5.15}$$

which we use in plotting a figure of a stationary breather.

Figure 4 shows the difference which the inclusion of cubic terms in the asymptotic expansion makes to the shape of a breather in a discrete generalized nonlinear Klein–Gordon equation. The top curve is the expansion up to $\mathcal{O}(\varepsilon^3)$ which we have derived here (5.13), the second curve is the $\mathcal{O}(\varepsilon^2)$ approximation and the smallest positive curve represents the leading-order approximation. At $t = \pi/\omega$ the variable ϕ takes its most negative values: the leading-order expansion is the one which is most negative at $x = 0$. The two-term

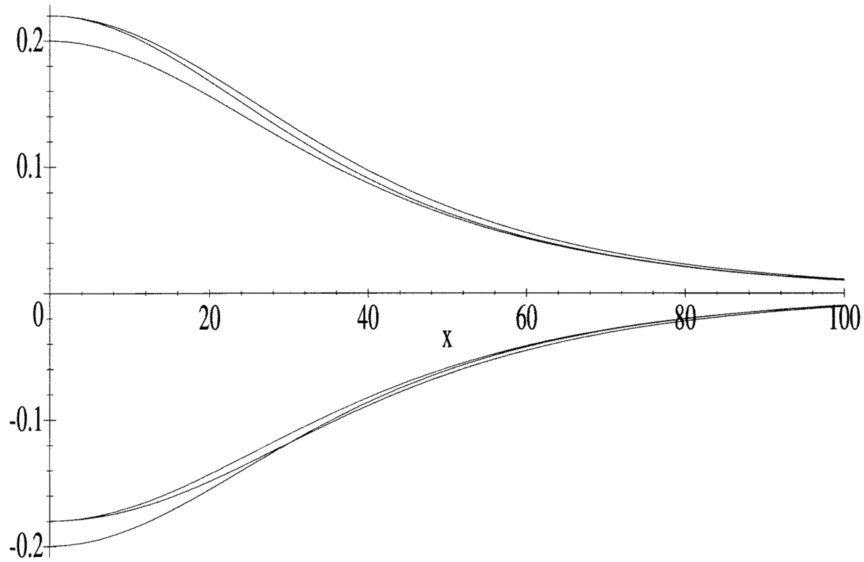

Figure 4. Plots of approximations to the breather at $t = 0$ and $t = \pi/\omega$ for the approximation up to third order in ε, up to second order, and the leading order term. The leading order term is exactly ± 0.2 at $x = 0$. The uppermost curve is the $\mathcal{O}(\varepsilon^3)$ approximation which at $t = \pi/\omega$ starts at -0.18 (when $x = 0$) and crosses the leading order term at $x = 30$. The two-term approximation is the least negative of the curves at $t = \pi/\omega$ and when $t = 0$ lies between the two positive curves. The parameter values used are $\varepsilon = 0.1$, $\Gamma = 0.236$, $A = 1.0$, $f = 1$, $h = 0$, $g = -0.05$, $\gamma_1 = 1.5$, $\gamma_2 = -1.166\,67$, $\gamma_3 = 0.625$ and $\gamma_4 = -0.258\,33$.

approximation is least negative, and the $\mathcal{O}(\varepsilon^3)$ approximation is coincident with the $\mathcal{O}(\varepsilon^2)$ expansion at $x = 0$, but then crosses the leading-order approximation and for larger x values is more negative than either of the others.

6. Discussion

In this paper we have shown how to calculate the differences that discreteness makes to the shape of a breather in a DSG lattice and in a general nonlinear Klein–Gordon lattice. The methods used have required the derivation of highly accurate quasi-continuum approximations using Padé approximates to rewrite the discrete difference operator in terms of spatial derivatives. This enables the system of coupled ordinary differential equations to be approximated by a single PDE which has the form of a perturbed continuum Klein–Gordon equation. This, in turn is solved by using multiple time scales to derive a hierarchy of perturbed nonlinear Schrodinger equations. The solution of these requires the imposition of secularity conditions. In general, breather modes do not form exact solutions to perturbed sine–Gordon equations, but they are observed to be extremely long-lived oscillations. Detailed knowledge of the breather's form is thus crucial to the understanding of the large-time evolution of such systems.

In sections 2 and 3 we have analysed the DSG equation using quasi-continuum expansions and multiple-scales techniques. The usual continuum expansion, which keeps only the first two spatial derivatives, is solved using two time scales and one length scale and leads to the same solution as for the stationary breather in the SG system. Only when the breather moves does the lattice structure underlying the DSG system cause any difference to the shape of the breather at leading order—these leading-order effects were found by Remoissenet [7].

The analysis presented here extends the leading-order results by calculating the correction terms in the asymptotic expansion and showing how to calculate successive terms. To calculate the first correction term three time scales and two space scales are required. We have shown how to find and impose the secularity conditions necessary for these higher-order expansions to be solved. Differences between stationary breathers in the DSG and SG systems are then revealed. Our results agree with previous observations of breathers in the DSG system [13], namely that discreteness causes an increase in the frequency of oscillation and a reduction in the width of the breather if the height is kept the same in the two scenarios (DSG and SG).

PDEs from which these results were obtained were derived from the differential-difference equation by forming Padé approximations of the discrete difference operator in the manner used in earlier studies of lattice dynamics [10–12]. Various forms of Padé approximation all lead to the same expansion for the breather, but exhibited differences in their approximation of the dispersion relation for small amplitude linear waves. The standard quasi-continuum approximation (corresponding to a (4,0) Padé approximate) has the unfortunate property of predicting an instability at large wavenumbers. The (4,2) Padé approximate is more accurate than (4,0) at small wavenumbers but has the same singularity at larger wavenumbers. The best qualitative approximation of the dispersion relation is obtained by using the (2,2) Padé approximation which assigns real and finite frequencies to all wavenumbers—as the discrete dispersion relation does. However, the band which the predicted frequencies lie in is somewhat broader in the (2,2) Padé approximation than for the exact solution.

Although all of the more accurate quasi-continuum approximations have yielded the same breather solution, the behaviour of small-amplitude linear waves is seen to differ. This is indicative of possible wider differences in the systems; for example, the manner in which breathers interact with each other, or with kinks, or with small-amplitude linear waves could also differ. This is particularly important since it is known that the DSG equation is not integrable and so the nonlinear modes (breathers and kinks) do not travel freely through the lattice—rather they shed radiation in the form of small-amplitude linear waves into the lattice. Analysis of the dynamics of such interactions needs to be undertaken with great care since simple continuum approximations such as the SG and the (4,0) Padé approximation are not the best available if one aims to analyse interactions of nonlinear modes using continuum techniques.

The Padé approximation technique was then applied to a generalized discrete nonlinear Klein–Gordon lattice with non-symmetric potential. This was derived from a coupled chain model with second-neighbour interactions and diagonal interactions between the two chains. Again the (2,2) Padé approximate gave qualitatively the best approximation to the dispersion relation of the lattice.

The nonlinear quasi-continuum PDE was solved using multiple-time-scale asymptotics, again with three time scales and two space scales. In this more complicated model, as in the simpler DSG case, the leading-order calculation of a static breather shows no differences in dynamics or shape from a continuum breather. As with modified KdV equations [4], differences are found at a higher order, and the analysis presented here enables alterations to the frequency and spatial shape to be calculated. After deriving and imposing the necessary secularity conditions, higher-order explicit approximations for the breather modes were derived. The advantage which this method has over the variational methods used earlier [13] is that the current method determines the differences in shape caused by the discrete nature of underlying space dimension. The price we pay is that the solutions generated here are valid only in the small-amplitude limit, so they are unlikely to provide an explanation for the pinning of the large-amplitude breathers.

One question which this analysis does help to answer is 'could breathers exist in a lattice where the parameter $\Delta_2 = 0$?' This could occur if second-neighbour interactions were competitive ($g < 0$), which would imply $\Delta_4 < 0$ and hence the stability of the zero solution. The dispersion relation is then very flat near $k = 0$, since $\omega^2 \sim \Gamma^2 + \mathcal{O}(k^4)$, but there still exists a band of frequencies below the linear waves. However, our analysis shows that breathers of the expected form are not possible as the limit $\Delta_2 \to 0$ in (5.12) is clearly singular. In a more rigorous analysis of the possible existence of breathers in this lattice, we consider other scalings for the variables $x_1, t_2 \ldots$, the correct scalings are then $x_1 = \varepsilon^{1/2}x$, $t_2 = \varepsilon^2 t$, which yields the equation

$$2\mathrm{i}\Gamma F_{1,t_2} = F_{1,xxxx} + K|F_1|^2 F_1 \tag{6.1}$$

in place of the NLS equation at $\mathcal{O}(\varepsilon\, \mathrm{e}^{\mathrm{i}\Gamma t_0})$. A search for separable solutions to this equation suggests that there are no solutions which decay as $x \to \pm\infty$.

Our generalization of the discrete nonlinear Klein–Gordon equation allows a novel type of breather solution. In cases where $\Delta_2 < 0$ the dispersion relation shows that the wave with number $k = 0$ has a frequency which is a local maximum. Thus there is no frequency gap below this but nonlinear waves with a larger frequency are possible.

If $g < 0$ then $\Delta_2 = f - h + 4g < 0$ automatically implies $\Delta_4 = f - h + 16g < 0$ and so the instability caused by the negative coefficient of the second spatial derivative is stabilized by the presence of a negative fourth derivative. Provided that $\Gamma^2 > -\Delta_2^2/4g$ and $\Gamma^2 > 16g - 4\Delta_2$, the system of ordinary differential equations is stable in the sense that all wavenumbers have real frequencies. The more accurate quasi-continuum approximations then give well-posed PDEs even though the standard continuum approximation is ill-posed. If $\gamma_2 < -\frac{10}{9}\gamma_1^2$ then the resulting nonlinear Schrödinger equation has a bright soliton solution and the breather's frequency lies above $\omega_0 = \Gamma$. (The case of $\Delta_2 < 0$ with $g > 0$ is less likely to occur as this requires $h > k$ which implies that an atom's interaction with a neighbouring atom is stronger if the atom is on the other chain.) It may be argued that breather modes above the dispersion relation have more in common with 'gap solitons' than breathers, but in our case there is no optical branch of frequencies above the region where solitons exist. Whether such modes are exact solutions of the kinetic equations remains an open problem as does their stability; if they are proven to exist, there is then the question of what happens to this branch of solutions as the amplitude is increased.

In summary this paper has addressed the question of finding highly accurate approximations to stationary breathers in Klein–Gordon chains. The reason for concentrating on stationary breathers is that the standard continuum approximation reveals no difference between breathers in the continuous and discrete versions of these modes. The more detailed calculations carried out here reveals the differences which an underlying discrete spatial structure imposes on the shape of breathers. The calculations require a multiple-scales analysis, which we have generalized from well known leading-order calculations carried out previously. When higher-order correction terms are required, secularity conditions need to be imposed, and here we have found the necessary conditions and solved the resulting equations. In applying the techniques to two coupled chains with generalized interactions, we have uncovered some new and intriguing phenomena.

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