Combined breathing–kink modes in the FPU lattice

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Combined breather–kink modes have been observed in several systems. Here we show that in the FPU lattice, small amplitude breathing–kink modes are three-soliton solutions of an associated mKdV equation. Since this is integrable, the modes can be constructed using the Bäcklund transform. As well as finding explicit solutions, we consider the stability of the combined mode using variational techniques and illustrate stability for some parameter values and instability for others.

FPU lattice. However, this calculation is not accurate for times greater than $O(\varepsilon^{-2})$, where $\varepsilon$ is the amplitude of the mode. Wang [4] finds that the cubic anharmonicity of lattices causes high-frequency modes to suffer a long wavelength modulation. Simulations confirming this effect exhibit breathing–kink modes. In [7], Flach and Gorbach use numerical techniques to construct breather solutions of the FPU problem and analyse their stability. Fig. 8 of [7] shows a highly discrete combined breather–kink mode, centred between lattice sites, calculated by continuation techniques to a non-small amplitude. Floquet analysis shows the mode is unstable. Fig. 14 of [7] also shows two families of combined breather–kink modes, both closer to the continuum limit (small amplitude, and spread over many lattice sites). Whilst the energy of one family of solutions vanishes as its frequency approaches the phonon band, that of the other does not. Iooss and James [8] consider the problem of breathers in FPU–Klein–Gordon lattices and, from a centre-manifold reduction, deduce that breathers must be superimposed on an oscillatory quasiperiodic tail, whose amplitude is exponentially small.

The existence of travelling waves in the FPU lattice was established by Friesecke and Wattis [9], and that of breathers by Aubry [10] and Aubry et al. [11]. The FPU lattice is not integrable, so the nonlinear localised modes of the two types are not expected to interact elastically. The rigorous existence of breathers coupled to a static deformation of the lattice was shown by Livi et al. in [12] for the case of a diatomic FPU lattice. It is natural to consider the breather as the ac component since it oscillates in time and in space, and the kink component is then akin to an induced dc component of the nonlinear mode. The presence of this dc component

1. Introduction

Moving breathing–kink modes have been observed in several numerical simulations; see for instance, the work of Bickham et al. [1], Gaididei et al. [2], Huang et al. [3] and Wang [4]. In this paper we provide an explanation for the phenomenon in terms of an asymptotic reduction of the governing lattice equations to the mKdV equation, which is an integrable system known to support both travelling kink and breather solutions. Remarkably, Bickham et al. [1] and Huang et al. [3] simultaneously published work on moving breathing–kink modes in an FPU system with cubic and quartic anharmonicity. Whilst Bickham et al. used a rotating wave approximation to generate their modes, Huang et al. used a small amplitude asymptotic reduction. However, since they attack the problem directly, their solution ansatz required two leading order terms, one for the kink component ($\phi$, say) and one for the breather component ($\psi$, say); the latter is determined by a nonlinear Schrödinger equation and the former by $\partial_t \phi \propto |\psi|^2$. They call the resulting combined modes ‘asymmetric intrinsic localised modes’. A similar approach is taken by Flytzanis et al. [5], who also numerically study the collision of such modes and find them to be elastic.

The work of Butt and Wattis [6] uses a simpler asymptotic ansatz to show how breather–kink modes might arise in the

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is due to the phonon band including arbitrarily small frequencies; such a band is referred to as acoustic. The diatomic FPU lattice has two bands—an acoustic one and an optical one. In [13], Flach et al. consider a two-dimensional lattice which supports breather-type modes which exhibit both ac and dc components.

The interactions of solitary waves has been studied in integrable systems, for which analytical methods as well as numerical techniques are available for explaining the findings. Kevrekidis et al. [14] studied the stability of two-soliton solutions of the positive mKdV equation and found them to be stable. However, the periodic array of breather solutions in such a system was found to be unstable. Chow et al. [15] analysed the interaction of a solitary wave with a breather in the extended KdV system (effectively, a linear combination of KdV and mKdV equations). Since this system is integrable, one expects soliton waveforms to regain their shape after a collision, only suffering a phase shift, as is observed in their simulations.

Gaididei et al. [2] considered a two-dimensional lattice with in-plane displacements, and reduced the system to two coupled nonlinear Schrödinger equations. They found that both components of the displacement vector have the form of moving breather–kink modes which appear to travel through the lattice without suffering any appreciable loss of energy; they also find modes in which one displacement has the form of a moving breather–kink mode and the other is a classical breather; see Figs. 2, 3 and 8 of [2]. Kourakis and Shukla have noted the existence of breather–kink modes in models of dusty plasma crystals, though they named them ‘asymmetric bright envelope solutions’; see Figs. 5b and 6 of [16,17] respectively.

The purpose of this paper is to show the connection between breather–kink modes in the one-dimensional FPU lattice and the mKdV equation. This explains how such modes may be constructed, and gives a more thorough justification of their existence than can be shown by asymptotic approximations. It also explains their stability under collisions. The reduction from the FPU form to the mKdV equation is given in Section 2. In Section 3 we show how to use the Bäcklund transform to construct two-soliton and three-soliton solutions of the mKdV equation. These results are illustrated in Section 4 where the stability of the modes is discussed; finally conclusions are drawn in Section 5.

2. Small wavenumber asymptotics for breathing–kink modes

2.1. Formulation

To investigate the asymptotic moving breather–kink mode found in [6] we perform a multiple-scales expansion for the one-dimensional FPU form

$$J_{\text{FPU}} = \sum_n \frac{1}{n^2} p_n^2 + V(q_{n+1} - q_n),$$

where $V(\phi) = \frac{1}{2} \phi^2 + \frac{1}{2b} \phi^4$ and $b > 0$. This implies

$$\frac{d^2 q_n}{dt^2} = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}),$$

or, under the transformation $\phi_n = q_{n+1} - q_n$,

$$\frac{d^2 \phi_n}{dt^2} = V'(\phi_{n+1}) - 2V'(\phi_n) + V'(\phi_{n-1}),$$

where $V'(\phi) = \phi + b\phi^3$.

Travelling wave solutions of (2.2) have the form of a kink, whereas in the $\phi_n$-variables (2.3) the shape is that of a pulse. Breather solutions of (2.2) correspond to breather solutions of (2.3).

However, the reverse is not necessarily true. Since $q_n = \sum_{k=-\infty}^{n-1} \phi_k$, the quantity $q_n$ is only a classical breather (with zero boundary conditions applying as $n \to \pm\infty$) if the condition $\sum_{k=-\infty}^{n-1} \phi_k = 0$ holds. Whilst this may be true, it is also possible that this sum (which equals $q_\infty - q_{-\infty}$) is non-zero; it is these modes with nonzero differences $q_\infty - q_{-\infty}$ that we are concerned with in this paper.

2.2. Asymptotic reduction to the mKdV equation

The system (2.3) has a dispersion relation ($\phi_\infty = e^{i\kappa_j k - \Omega_j t}$ for $\epsilon \ll 1$)

$$\omega = \pm 2\sin \left( \frac{1}{2} k \right),$$

(2.4)

In the limit of small $k$, this gives $\omega \sim k$; hence the term $e^{i\kappa_j k - \Omega_j t}$ ceases to be discrete in space and vary over $\mathcal{O}(1)$ timescales, and, instead, becomes part of the long timescale, large space-scale expansion. It is this limit that we are concerned with here. Hence we assume

$$\phi_n = \epsilon F(x_1, t_1, x_2, t_2, \ldots) + \epsilon^2 G(x_1, t_1, x_2, t_2, \ldots) + \epsilon^3 H(x_1, t_1, x_2, t_2, \ldots) + \ldots,$$

(2.5)

where $x_0 = \epsilon n$, $t_0 = \epsilon t$, $(j \in \mathbb{N})$,

and we neglect any dependence on the $x_0 = n$ or $t_0 = t$ scales.

Eq. (2.5) together with (2.6) implies

$$\phi_{n+1} = \epsilon^2 F_{n+1} + 2\epsilon^3 F_{n+2} + \epsilon^4 G_{n+1} + \epsilon^5 G_{n+2} + 2\epsilon^3 F_{n+1} + 2\epsilon^4 F_{n+2} + \epsilon^5 H + \mathcal{O}(\epsilon^6),$$

(2.7)

$$\phi_{n-1} = \epsilon^2 F_{n-1} + \epsilon^3 F_{n-1} + \epsilon^4 G_{n-1} + \epsilon^5 G_{n-1} + \epsilon^6 H_{n-1} + \mathcal{O}(\epsilon^6),$$

(2.8)

by equating terms at equal orders of $\epsilon$, we find the following equations.

At $\mathcal{O}(\epsilon^2)$:

$$F_{n+1} = 2F_{n+2} + 2G_{n+1} + \mathcal{O}(\epsilon^2),$$

(2.9)

and hence $F = F(x_1 - t_1) + \mathcal{O}(\epsilon^2)$. Since we are considering copropagating waves, we put $F = 0$ and focus on $\epsilon$. Putting $F \neq 0$ and $F \neq 0$ would allow analysis of the head-on collisions of waves. At $\mathcal{O}(\epsilon^4)$:

$$2F_{n+2} + 2G_{n+1} = 2F_{n+2} + 2G_{n+1},$$

(2.10)

and we assume that $G$ satisfies the same equation as $F$, and hence $F_{n+2} = F_{n+2}$. Since $F = F(x_1 - t_1, x_2, t_2)$ we find $F_{n+2} = F_{n+2}$ which has travelling wave solutions of the form $F = F(x_1 - t_1, x_2, t_2)$ this dependence on the $(x_2, t_2)$ scales is of the same form as the dependence on $(x_1, t_1)$, so we will absorb it into the leading order behaviour, and assume that $F$ evolves only due to the $(x_1, t_1)$ argument and through the $(t_1, t_2)$ and longer timescales.
The effect of the asymptotic reduction on the variational pulses in \( F \) gives the positive modified Korteweg–de Vries (mKdV) equation as for \( p \):

\[
2F_{t1t1} + F_{zz} + 2G_{t1z} + H_{t11} = \frac{1}{12} F_{x1x1x1} + F_{x2x2} + 3bF^2 F_{x1} + 6bF^3 F_{x1x1}.
\]

As for \( G \), we assume that \( H \) satisfies \( H_{t11} = H_{t1} \), that \( G_{t1z} = G_{x1z} \), and that \( F \) is independent of \( x_2 \). Simplifying (2.11), we find

\[
2F_{t1t1} = \frac{1}{12} F_{x1x1x1} + 3bF^2 F_{x1} + 2F_{x1x1}.
\]

We are interested in the long time evolution of wave profiles on the \( x_1 \) scale. We now transform to moving wave coordinates, \( z = x_1 - t_1, \tau = t_1, T = t_1 + x_3 \), and \( Z = x_1 - t_3 \); hence

\[
2F_{\tau \tau} - 4F_{\tau z} = \frac{1}{12} F_{zzzz} + 3bF^2 F_{\tau}.
\]

If we assume the existence of a \( \tau \)-independent solution then this equation loses all dependence on \( z \), and can be integrated once to give the positive modified Korteweg–de Vries (mKdV) equation

\[
0 = 4F_{\tau} + \frac{1}{12} F_{zzzz} + 3bF^2 F_{\tau}.
\]

This equation has been widely studied, and its properties are described in a wide variety of textbooks, for example, Draizin and Johnson [18], Lamb [19], Ablowitz and Segur [20], Fordy [21], and Hirota [22]. The mKdV equation (2.14) is known [18] to have a moving breather solution of the form

\[
F_{\nu} = \frac{-2}{\sqrt{6b}} \tan^{-1} \left( \frac{F_{num}}{F_{den}} \right),
\]

\[
F_{num} = c \sin \left( \sqrt{6b} \left[ z + \frac{1}{8} bT (a^2 - 3c^2) + p \right] \right),
\]

\[
F_{den} = a \cosh \left( \sqrt{6b} \left[ z + \frac{1}{8} bT (3a^2 - c^2) + q \right] \right).
\]

Here \( a, c, p, q \) are arbitrary constants. This solution has \( \int_{-\infty}^{\infty} F_{\nu} dz = 0 \) and by judicious choices of \( a \) and \( c \) the breather can be made to move in either the positive or negative \( z \)-direction. However, Eq. (2.14) also has travelling pulses of the form

\[
F_{\nu} = \pm \sqrt{\frac{2v}{b}} \sech(4\sqrt{3v}(z - vT)),
\]

which satisfies \( \int_{-\infty}^{\infty} F_{\nu} dz = \pm \pi / \sqrt{6b} \); whilst this gives rise to pulses in \( F \) and \( \phi \), in the original \( q_1(t) \)-variables, it has a kink profile. Due to the form of (2.16), pulses only exist with \( v > 0 \) which implies that the velocity in the original variables \( (n, t) \) is \( 1 + e^\nu v \), so these pulse waves can only be superonic. Since the mKdV equation is odd in \( F \), once one solution is known, a second is automatically found by considering \( -F \). Thus, travelling pulses can be waves of elevation or of depression.

2.3. The effect of the asymptotic reduction on the variational formulation

From the variational formulation of the FPU lattice (2.1), we obtain an expression for the energy. We now apply the transformations \( \phi_{\nu} = q_{n+1} - q_n, \phi_{\nu} = \varepsilon F(x_1, t_1, \ldots) \) and \( F = W_{x1} \), where \( x_1 = \varepsilon \tilde{t}, t_1 = \varepsilon t, \) to the kinetic and potential energy components of (2.1). The potential energy \( U \) is given by

\[
U = \sum_n \left( \frac{1}{2} \phi_{\nu}^2 + \frac{1}{4} b \phi_{\nu}^4 \right)
\]

\[
\sim \int \frac{1}{2} W_{x1}^2 + \frac{1}{4} b \varepsilon^4 W_{x1}^4 dx_1,
\]

The calculation for the kinetic energy, \( \mathcal{J} \), is more complex. We Taylor expand about the mid-point of \( q_{n+1} \) and \( q_n \), obtaining \( q_{n+1} = q + \frac{1}{2} \varepsilon q_{x1} + \frac{1}{4} \varepsilon^2 q_{x1x1} + \frac{1}{24} \varepsilon^3 q_{x1x1x1} \) and \( q_n = q - \frac{1}{2} \varepsilon q_{x1} + \frac{1}{4} \varepsilon^2 q_{x1x1} + \frac{1}{24} \varepsilon^3 q_{x1x1x1} \), and then \( q_{n+1} - q_n = \varepsilon \phi_{\nu} + \frac{1}{24} \varepsilon^3 q_{x1x1x1} \). Since \( q_{n+1} - q_n = \phi_{\nu} = \varepsilon F \), we have \( \varepsilon F = \varepsilon F \left( q_{x1x1} + \frac{1}{24} \varepsilon^3 q_{x1x1x1} \right) \) and so \( \varepsilon q_{x1x1} \sim \varepsilon F - \frac{1}{24} \varepsilon^3 F \). Now using \( F = W_{x1} \) and integrating implies \( q \sim W - \frac{1}{24} \varepsilon^3 W_{x1} \). Thus

\[
\mathcal{J} = \sum_n \int \frac{1}{2} W_{x1}^2 + \frac{1}{24} \varepsilon^3 W_{x1}^2 dx_1.
\]

The latter stages of the calculation are due to \( \frac{\partial}{\partial \varepsilon} \varepsilon \phi_{\nu} + \frac{1}{3} \varepsilon \phi_{\nu} \), an integration by parts, and the substitution \( Z = x_1 - t_1, T = t_1 \). Hence we obtain the expression \( \mathcal{J} = \mathcal{J} + U: \)

\[
\varepsilon = \int \varepsilon W_{x1}^2 - \varepsilon^3 W_{x1} x_1 + \frac{1}{24} \varepsilon^3 W_{x1}^2 dz,
\]

for the energy of the mKdV approximation to the FPU lattice (2.1), and the Lagrangian of this system is given by \( \mathcal{L} = \mathcal{J} - U: \)

\[
\mathcal{L} = \int \frac{1}{24} \varepsilon^3 W_{x1}^2 - \varepsilon W_{x1} x_1 - \frac{1}{24} \varepsilon^3 W_{x1}^2 dz.
\]

It can easily be verified that use of the Euler–Lagrange equations, together with the substitution \( F = W_{x1} \), leads from (2.20) to (2.14). This provides a variational formulation different from that usually presented, which is based on the Hamiltonian density

\[
\mathcal{H}_{mKdV} = \frac{1}{2} u_t^2 - \frac{1}{4} u_x^4,
\]

whence the Euler–Lagrange equation implies

\[
u_t = \frac{\partial}{\partial \varepsilon} \left( \frac{\partial \mathcal{H}}{\partial u} \right) = -6u u_x - u_{xxx}.
\]

The leading order \( (\varepsilon) \) expression for the energy (2.19) is simply \( I_2 = \int F^2 dz \), which is the second conserved quantity for the mKdV system (2.14), and is well-known to have an infinite hierarchy of conserved quantities (others at the start of the sequence include the mass \( I_1 = \int F dz \) and the Hamiltonian \( I_3 = \int F^2 - 6bF^4 dz \)).

3. Bäcklund transform analysis

3.1. One-soliton solutions

In this section we transform (2.14) using \( x = z, t = \frac{1}{\varepsilon} T \), and \( u = \varepsilon W_{x1} \). We define

\[
P = u_t + 6u^2 u_x + u_{xxx}, \quad Q = w_t + 2w_x^2 + w_{xxx},
\]

so the positive mKdV equation (2.14) becomes \( P = 0 \), and under the substitution \( u = w \), we have \( P = Q \). This \( w \)-formulation is used so that we can make use of the Bäcklund transform for the mKdV equation [19,23], which is

\[
(w_1 + w_3) = 2k_1 \sin(w_1 - w),
\]

\[
(w_1 + w_3) = -2k_1 [(u_1x - u_x) \cos(w_1 - w) + (u_t + u_x) \sin(w_1 - w)].
\]

Here, \( w \) is one solution of the mKdV equation, which we assume is known (for example, \( w = 0 \)). The second solution, \( w_1 \), we aim
to construct by integrating the two equations (3.2)–(3.3) to find a general one-soliton solution which depends on the arbitrary parameter $k_1$. We assume that by taking different values of this parameter it is possible to construct a family of solutions.

Starting from the trivial solution with $w = 0$, we integrate (3.2), which is $w_{1,x} = 2k_1 \sin w_1$, to obtain log tan $\frac{1}{2} w_1 = 2k_1 x + C_0(t)$ for some function $C_0(t)$. With $w = 0$, Eq. (3.3) reduces to

$$w_{1,1} = -2k_1 [w_{1,xx} \cos w_1 + w_{1,x}^2 \sin w_1],$$

which can equivalently be written as

$$\tan \frac{1}{2} (w_{12} - w) = \frac{k_1 + k_2}{k_1 - k_2} \frac{1}{2} (w_{12} - w_1).$$

(3.14)

Noting that $w = 0$ and using the solutions (3.6), and the trigonometric formula for expanding tan$(A + B)$, this solution can be expressed as

$$w_{12} = 2 \tan^{-1} \left( \frac{k_1 + k_2}{k_1 - k_2} \frac{e^{w_2} - e^{w_1}}{1 + e^{w_1}e^{w_2}} \right),$$

(3.15)

or

$$\tan \frac{1}{2} w_{12} = \frac{1}{2} \left( \frac{k_1 + k_2}{k_1 - k_2} \sin \frac{1}{2} (\theta_2 - \theta_1) - \cosh \frac{1}{2} (\theta_1 + \theta_2) \right).$$

(3.16)

In a similar way, it is possible to construct the solutions $w_{13}$ from $w_{11}$ and $w_3$ and $w = 0$, and also $w_{23}$ from $w_2$, $w_3$ and $w = 0$ using (3.6). For $w_{12}$ to be real, there are restrictions on $k_1$, $k_2$, $x_1$, $x_2$. When the parameters are complex, the formula (3.15) still provides a solution of the mKdV equation, and can be used to construct further multi-soliton solutions of the mKdV equation. Combining two complex soliton solutions using the Bäcklund transform can make a real multi-soliton solution; for example if $k_2 = k_1^* + \varepsilon$ and $x_2 = x_1^* + \varepsilon x_1$, then $w_{12} \in \mathbb{R}$ even though $w_{11}$, $w_{22} \in \mathbb{C}$ (where $x, t \in \mathbb{R}$).

A real breather is plotted in Fig. 1. The velocity of the breather envelope can be deduced from the form of the second denominator of (3.15). We write $k_{1,2} = \mu \pm \nu i$; then

$$\theta_1 + \theta_2 = 4\mu x - 16(\mu^2 - 3\nu^2)t - 2(\mu + \nu)x_1 - 2(\mu - \nu)x_2,$$

(3.17)

and hence the breather velocity is $4(\mu^2 - 3\nu^2)$, which in the case plotted gives a speed of 4. The time period for the internal mode of oscillation is given by the corresponding numerator, and is given by $2\pi / 8\nu (3\mu^2 - \nu^2) \approx 0.0015$.

3.3. Three-soliton solutions

Three-soliton solutions can be constructed in a way similar to that described in the previous subsection. We take (3.13) and replace $w_{12}$ with $w_{12,3}$, $w_{12}$ by $w_{12,2}$, $w_2$ by $w_2$, and $w$ by $w_2$, to obtain

$$w_{123} = w_2 + 2 \tan^{-1} \left( \frac{k_1 + k_3}{k_1 - k_3} \frac{1}{2} (w_{23} - w_1) \right),$$

(3.18)

or

$$\tan \frac{1}{2} (w_{123} - w_2) = \frac{1}{2} \left( \frac{k_1 + k_3}{k_1 - k_3} \frac{w_{num}}{w_{den}} \right),$$

(3.19)

This leads to

$$w_{123} = w_2 + 2 \tan^{-1} \left( \frac{k_1 + k_3}{k_1 - k_3} \frac{w_{num}}{w_{den}} \right),$$

(3.20)

where

$$w_{num} = (k_2 + k_3)(k_1 - k_3) \sinh \frac{\theta_2}{\theta_1 + \theta_2} \sinh \frac{\theta_1 + \theta_2}{2},$$

$$- (k_1 + k_3)(k_2 - k_3) \sinh \frac{\theta_2}{\theta_1 + \theta_2} \cosh \frac{\theta_1 + \theta_2}{2},$$

$$w_{den} = (k_2 - k_3)(k_1 - k_3) \cosh \frac{\theta_2}{\theta_1 + \theta_2} \cosh \frac{\theta_1 + \theta_2}{2} + (k_2 + k_3)(k_1 + k_2) \sinh \frac{\theta_2}{\theta_1 + \theta_2} \cosh \frac{\theta_1 + \theta_2}{2}.$$
Fig. 1. Illustration of the two-soliton solution (3.15) in the case \( k_1,2 = 7 \pm 4i \), \( x_1 = 0 = x_2 \). Left: the solid line corresponds to \( t = 0 \), the dashed line to \( t = 0.27 \), and the dash–dotted line to intermediate times of \( t = 0.045, 0.09, 0.135, 0.18, 0.225 \). Right: 3D plot over the same scales.

Fig. 2. Illustration of how three separate one-soliton solutions can be combined using Bäcklund transforms to construct a three-soliton solution, via the construction of two two-soliton solutions.

ensure that \( w_{123} \) is real—although, when constructing the three-soliton solution, we do not require that \( w_{12} \) and \( w_{23} \) are real.

An example plot of (3.20) is shown in Fig. 3. To construct this combined breather–kink mode which remains co-localised we choose \( k_{1,2} = 7 \pm 4i \) which gives \( w_{12} \) as a breather which travels at speed \( 4[\text{Re}(k)^2 - 3\text{Im}(k)^2] = 4 \). Then we choose a real value for \( k_3 \) which will give a kink which travels at the same speed—this is given by \( 4k_3^2 \); we choose \( k_3 = -1 \). The phase shifts \( x_1, x_2, x_3 \) are all chosen to be zero; hence the breather is located at the centre of the kink. Note the different forms of the solution when the wave is symmetric and centred at \( x = -24 \) and \( x = 0 \). The time period of the internal mode is as given at the end of Section 3.2, namely \( 2\pi/4192 \approx 0.001499 \). A plot of this internal motion over one period is shown in Fig. 4; note that the time interval is so short that the motion of the kink is not observable.

When \( k_{1,2} = \mu \pm vi \) and \( k_3 \ll \mu, v \), the breather component is significantly narrower than the kink component, as shown in Fig. 4. However, when \( v \ll \mu, k_3 \) then the breather widens the kink significantly, as shown in Fig. 5. In this case, the kink moves a significant amount during the time period of the breather’s oscillation.

4. Stability

In the above section we have shown that there is a three-soliton solution in which the kink and breather remain together (‘co-localised’). However, to determine whether we would expect to observe such a solution in a lattice simulation, we should investigate the stability of these solutions.

In Figs. 6 and 7, we illustrate the case where \( k_{1,2} = 13 \pm 4i \); such a breather \( (w_{12}) \) travels at speed \( v = 484 \). There are two kinks which travel at this speed, corresponding to \( k_3 = \pm 11 \). Fig. 6 shows the results for \( k = -11 \) whilst Fig. 7 illustrates the case \( k_3 = +11 \). In each figure we show small inner graphs which illustrate the form of the breather–kink modes when maximally overlapped \( (x_3 = 0) \) and when well-separated \( (x_3 = \pm 0.5 \) for \( k_3 = -11 \) and \( x_3 = \pm 0.12 \) for \( k_3 = +11 \)). The waveforms in \( w \)-variables are illustrated uppermost in each pair, the lower curve showing the shape in \( u \).
Fig. 4. Illustration of the three-soliton solution (3.20) in the case $k_1, k_2 = 7 \pm 4i$, $k_3 = -1$, $x_1 = x_2 = x_3$. Left: the solution is plotted at times $t = 9.00000$ (solid line), 9.00021, 9.00042, 9.00063, 9.00084, 9.00105, 9.00126, 9.00147. Right: 3D plot over the same ranges of $x$ and $t$.

Fig. 5. Illustration of the three-soliton solution (3.20) in the case $k_1, k_2 = 13 \pm 4i$, $k_3 = 11$, $x_1 = x_2 = x_3$. Left: the solution is plotted at times $t = -0.0002$ (solid line), $-0.0001$ (dash–dotted), 0 (dotted), 0.0001 (dashed), 0.0002 (solid). Right: 3D plot over the same scales of space and time.

Fig. 6. Illustration of the energy $E(x_3) - E(0)$ plotted against $x_3$, where $u = w_{123,x}$ and $E(x_3) = \int u^2 \, dx$ is the energy of the breather–kink mode as a function of $x_3$ (outer plot, for $-0.5 \leq x_3 \leq 0.5$). Three pairs of internal plots show $w_{123}$ (the upper of each pair) and $u = w_{123,x}$ (lower) for $-1.5 \leq x \leq 1.5$ for the case $k_{1,2} = 13 \pm 4i$, $k_3 = -11$. The left (right) pairs of graphs show the case $x_3 = -0.5$ ($x_3 = +0.5$), whilst the central pair shows $x_3 = 0$; in each case $x_1 = x_2 = 0$ and $t = 0$.

The main curve is a plot of the energy difference, $E(x_3) - E(0)$, given by (2.19) plotted against $x_3$. The reason for subtracting $E(0)$ is the size of all energies in comparison with the differences; for the example plotted, we have $E_{x_3=0} \approx 5.9 \times 10^6$. These calculations have been performed in Matlab using digits $\approx 20$.

In the case $k_3 < 0$ the energy reaches a maximum when the kink and breather are superposed (Fig. 6), suggesting that the combined breather–kink waveform requires more energy than the separated waveforms. We might expect such a combined wave to decay as the components of the wave slowly drift apart, releasing the excess energy as radiation. Since the energy differences are small, we expect the timescale over which the waves to separate to be slow in the mKdV system; the timescale in the original FPU problem will be extremely slow since it is related to the mKdV timescale through a rescaling with a factor of $O(\varepsilon^{-3})$. Hence the unstable breather–kink waveform may be described as metastable, since its decay is so slow.

When $k_3 > 0$, the overlapped waveform has lower energy than the separated forms (Fig. 7), suggesting that the combined mode is stable. We note that these effects are extremely small, since the energy differences are $O(1)$ in both cases ($k_3 > 0$ and $k_3 < 0$; in fact 0.8 and 0.0035 respectively) whilst the total energy in the
combined mode is $\delta \approx 5.9 \times 10^6$. We note that the potential well for $k_3 > 0$ is significantly deeper than the peak for $k_3 < 0$; however the width is much reduced (a half-height width of $\Delta x_3 < 0.01$ for $k_3 > 0$ as opposed to $\Delta x_3 \approx 0.2$ for $k_3 < 0$).

5. Conclusions

Through asymptotic reductions of the $\beta$–FPU lattice to the mKdV equation we have shown that breathing–kink modes observed in the former can be constructed as three-soliton solutions of the latter via the Bäcklund transform. This gives a method for constructing explicit approximations for them, and explains why they are so robust under collisions with each other and other solitary wave solutions. It also enables us to analyse their stability in the longer term and, by explicitly constructing mixed modes in which the breather and the kink travel at identical speeds, to show that the combined breather–kink mode can exist for an arbitrarily long time.

Whilst the mKdV breather can move in either direction, the kink can propagate only with a positive velocity; hence moving breather–kink modes can only exist with positive velocities. Carrying these results over to the FPU lattice yields the implication that moving breather–kink modes are supersonic modes. Since there is a two-parameter family of kinks (speed and phase) and a four-parameter family of breathers (two phases, group velocity and phase velocity), requiring the two to travel at the same speed still leaves three phases and two other parameters free. We find that varying these changes the relative widths of the breather and the kink, giving rise to a wide variety of waveforms (Figs. 3–5).

We have shown how the asymptotic reduction from the FPU form to the mKdV equation acts on the variational formulation of the problem, and hence found that the second conserved quantity of the mKdV equation corresponds to the FPU energy. This enables us to comment on the stability of the combined three-soliton wave as a function of the relative displacement of the breather and the kink. For certain parameters, the combined wave is stable, having a lower energy than the separated breather and kink (Fig. 7). However, for other parameter values, the combined mode is a local maximum (Fig. 6), suggesting that there would be energy released as the waves separated, and hence the mode might be expected to be unstable.

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