Variational approximations to breather modes in the discrete sine-Gordon equation

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Abstract

Long-lived breather-like modes have been observed in the numerical simulations of discrete sine-Gordon systems. However, little analytical work has been carried out on these systems. We show how to use the Variational form of nonlinear Klein–Gordon equations to find corrections to breather modes caused by discreteness.

1. Introduction

The Discrete sine-Gordon equation (DSG) occurs in many derivations of physical processes, and has consequently inspired many numerical simulations [1–4]. The passage to the continuum sine-Gordon equation (SG) is not always a good approximation. In some applications it is the propagation of travelling waves that is of main interest (e.g. long Josephson junctions [5–7]), in others, it are breather modes (e.g. DNA [8] or emission spectra of certain chemicals [9]). Hence the need to develop tools to examine breather modes in systems where discreteness is left in the mathematical model. This paper details one method of achieving this. An earlier paper [10] described the use of continuum methods in describing the shape of DSG breathers.

Most recent work on breathers in discrete systems concentrates on stationary breathers, as we shall do here. The method presented here should generalise to moving breathers, with some more work. (It is hoped to do this later.) However once a breather starts to move in a spatially modulated system, we expect to observe the discreteness causing much greater effects; these effects are harder to analyse for a breather than for a slowly moving kink (for example) due to the fact that a well-defined Peierls–Nabarro Potential exists for the latter but not for the former.

Numerical work suggests that both kinks and breathers in DSG suffer losses (Peyrard and Kruskal [11], Boesch and Peyrard [2], Dauxois and Peyrard [3], Flach and Willis [4]). These losses are small enough for the breather still to be considered an important nonlinear localised mode, worthy of further study.

The method presented here exploits the variational form of nonlinear Klein–Gordon equations – namely that the trajectory the system follows in phase space is a critical point of the action functional. We make use of this fact by assuming a solution for the breather which includes undetermined parameters. These parameters are...
then chosen in such a way as to make the action critical. This uses the same ideas as in [12] – a combination of ideas from the Calculus of Variations and finite element methods to obtain an analytic approximation. The method provides the most accurate approximation when applied to small amplitude, high-frequency breathers.

We start by considering SG in the form

$$\phi_{tt} = \phi_{xx} - \Gamma^2 \sin \phi,$$

(1.1)
we leave in a length and time scale to allow comparison with results from the DSG derived later on. In this form, the stationary breather is parameterised by $\mu$ by

$$\phi(x, t) = 4 \tan^{-1} \left( \frac{\tan(\mu)}{\cosh(\Gamma x \sin \mu)} \right),$$

(1.2)

The form of DSG which we study here is

$$\frac{d^2 \phi_n}{dt^2} = \phi_{n+1} - 2 \phi_n + \phi_{n-1} - \Gamma^2 \sin \phi_n,$$

(1.3)
$\Gamma$ cannot be removed by rescaling since the discreteness imposes a length scale on the system.

2. Variational approach to breathers in DSG

We rely on the theory of continuous Lagrangian and Hamiltonian systems as described, for instance by Goldstein [13]. Briefly, we note that the Lagrangian density is obtained from the difference of the kinetic and potential energies ($\mathcal{L}[\phi] = T - V$). The Lagrangian is then the spatial integral of this density ($L[\phi] = \int \mathcal{L}[\phi] \, dx$) and the action is the time integral of the Lagrangian ($S[\phi] = \int L[\phi] \, dt = \int \int \mathcal{L}[\phi] \, dx \, dt$). Hamilton’s Principal states that the equations of motion are determined by critical points of the action ($\delta S[\phi] = 0$), the Euler–Lagrange equations lead from this condition to the equation of motion.

Our method of approximation follows this recipe, until the critical points are to be calculated. At this stage we insert an assumed form for the wave $\phi(x, t; \mu)$, which contains three as yet undetermined parameters (represented by the vector $\mu$). The action is then calculated and two of the parameters related to the third by forcing the function $\phi(x, t, \mu)$ to be a critical point of the action functional.

As we have already seen, there is an exact representation of the breather mode in SG (1.2). The SG equation (1.1) is derivable from the Lagrangian density

$$\mathcal{L}_{\text{SG}} = \frac{1}{2} \phi_t^2 - \frac{1}{2} \phi_x^2 - \Gamma^2 (1 - \cos \phi).$$

(2.1)

To investigate the effects that discreteness may cause, we write the DSG equation in its Lagrangian form

$$L = \sum_n \frac{1}{2} \phi_n^2 - \frac{1}{2} (\phi_{n+1} - \phi_n)^2 - \Gamma^2 (1 - \cos \phi_n),$$

(2.2)

which induces the (infinite) set of ODEs (1.3). We now form a continuum expansion: $n$ is replaced by a continuous space variable ($x$), the ODE system is then Taylor expanded,

$$\mathcal{L}[\phi] = \frac{1}{2} \phi_t^2 - \frac{1}{2} \phi_x^2 - \Gamma^2 [1 - \cos \phi] + \frac{1}{24} \phi_{xx}^2.$$

(2.3)
This expansion of the Lagrangian corresponds to the natural way of expanding the differential equation to form a PDE of fourth order (in space),

$$\phi_{tt} = \phi_{xx} - \Gamma^2 \sin \phi + \frac{1}{12} \phi_{xxxx}.$$
The fourth derivative term is a correction to SG which includes the leading order discreteness effects.

If the continuous variables are rescaled so that $\tau = \Gamma t$, $\xi = \Gamma x$, then the expansion that has been made can be seen to be an asymptotic expansion for small $\Gamma$, since in these variables the differential equation and Lagrangian take the form

$$\phi_{\tau \tau} = \phi_{\xi \xi} - \sin \phi + \frac{1}{12} \Gamma^2 \phi_{\xi \xi \xi \xi} + O(\Gamma^4), \quad (2.5)$$

$$L[\phi] = \frac{1}{2} \phi_{\tau}^2 - \frac{1}{2} \phi_{\xi}^2 - \left[ 1 - \cos \phi \right] + \frac{1}{24} \Gamma^2 \phi_{\xi \xi}^2 + O(\Gamma^4). \quad (2.6)$$

In order to find an approximation which tells something of the effect of discreteness on a breather, we generalise the SG breather in such a way that the integrals needed to calculate the action ($S[\phi] = \int \int L[\phi] dx dt$) are still explicitly calculable. We define

$$\phi(x,t) = 4 \tan^{-1} \left( \frac{\tan(\mu) \sin(\omega t)}{\cosh(\rho x)} \right). \quad (2.7)$$

In this formulation the variable $\omega$ represents the frequency of the breather, $\mu$ determines the amplitude of the oscillation, and $\rho$ sets a width scale for the oscillation.

In the continuum limit we have $\omega = \Gamma \cos \mu, \rho = \Gamma \sin \mu$. The breather forms a one-dimensional family of solutions to SG - here parameterised by $\mu$. We also expect a one-dimensional family of solutions when discreteness has been accounted for.

For the following calculations, the definitions

$$S(\mu, \omega, \rho; \Gamma) = \int \int L[\phi] dx dt = T - U - \Gamma^2 V + W, \quad (2.8)$$

are used. The results for these are

$$T = \frac{16 \pi \omega \mu \tan \mu}{\rho_\omega}, \quad U = \frac{16 \pi \rho}{\omega} \left( 1 - \mu \cot \mu \right),$$

$$V = \frac{16 \pi \sin^2 \mu}{\rho \omega}, \quad W = \frac{\pi \rho^3}{9 \omega^3 \sin^3 \mu} \left( 3 \mu \cos \mu - 3 \sin \mu + \sin^3 \mu + 6 \sin^5 \mu \right). \quad (2.9)$$

Note that in the derivation here, various scalings have taken place, and the quantity $H = T + U + \Gamma^2 V - W$ is not the energy of the system (1.3). ($H$ is the integral of the Hamiltonian over one complete time period; see (2.17) for how this relates to the energy.)

The two equations we shall use to find $\omega, \rho$ are derived from Hamilton's principle. Following the integration of the assumed form (2.7) over $x$ and $t$, $S$ depends only on the three parameters $\omega, \rho, \mu$. Hamilton's principle reformulates to

$$\frac{\partial S}{\partial \mu} = 0, \quad \frac{\partial S}{\partial \rho} = 0. \quad (2.10)$$
Written in this form the equations are deceptively simple. These equations will automatically be satisfied to \( \mathcal{O}(F) \) by \( \omega(\mu) = F \cos \mu \), and \( \rho(\mu) = F \sin \mu \), since the assumed solution forms an exact solution for the SG equation. But these solutions imply \( W \sim \mathcal{O}(F^2) \) and so there will be correcting terms of \( \mathcal{O}(F^3) \) to the functions \( \omega(\mu), \rho(\mu) \).

\[
\begin{align*}
\omega(\mu) &= F \cos \mu \left[ 1 + F^2 \omega_1(\mu) + \mathcal{O}(F^4) \right], \\
\rho(\mu) &= F \sin \mu \left[ 1 + F^2 \rho_1(\mu) + \mathcal{O}(F^4) \right],
\end{align*}
\] (2.11)

for some \( \mathcal{O}(1) \) functions \( \omega_1(\mu), \rho_1(\mu) \) to be determined. Substitution into (2.10) and expansion leads to

\[
\begin{align*}
\mu \cos \mu \omega_1(\mu) + (\sin \mu - \mu \cos \mu) \rho_1(\mu) &= \frac{1}{32} \left[ \mu \cos \mu - \sin \mu - \frac{1}{3} \sin^3 \mu + 2 \sin^5 \mu \right], \\
(\sin \mu \cos \mu + \mu) \omega_1(\mu) + (\sin \mu \cos \mu - \mu) \rho_1(\mu) &= \frac{1}{96} \left[ \mu + 2 \mu \cos^2 \mu - 3 \sin \mu \cos \mu - \frac{1}{4} \right].
\end{align*}
\] (2.12)

The solutions of this equation are not simple, but can easily be found and plotted.

\[
\begin{align*}
\omega_1(\mu) &= -\frac{\sin \mu}{\Delta(\mu)} \left\{ 2\mu^2 \cos \mu - \mu \sin \mu (1 - 10 \sin^2 \mu + 4 \sin^4 \mu) - \sin^2 \mu \cos \mu (1 + 10 \sin^2 \mu) \right\}, \\
\rho_1(\mu) &= -\frac{1}{\Delta(\mu)} \left\{ \mu^2 \sin 2\mu + \mu (3 - 5 \sin^2 \mu + 10 \sin^4 \mu - 4 \sin^6 \mu) \\
&\quad + \sin \mu \cos \mu (6 \sin^4 \mu + \sin^2 \mu - 3) \right\}, \\
\Delta(\mu) &= 48(2 \mu \cos 2\mu - \sin 2\mu).
\end{align*}
\] (2.13)

From Fig. 1 we see that the correction terms are not small in the limit \( \mu \to \frac{1}{2} \pi \) and so we should not expect any asymptotic sequence to be valid in this region. This is the region where the breather almost has enough energy to separate into two kinks travelling apart. Kinks in DSG behave quite differently to those in SG radiate phonons as they move (Peyrard and Kruskal [11]). This is what we start to see with large amplitude breathers.
The small $\mu$ region is the only one we shall consider in detail. Small amplitude breathers have small corrections, suggesting that these form long-lived modes in a DSG chain with small $\Gamma$. For small $\mu$, the asymptotic expansions for $\omega_1(\mu)$ and $\rho_1(\mu)$ are

$$
\omega_1(\mu) \sim \frac{7\mu^4}{360} - \frac{211\mu^6}{37800} + O(\mu^8), \quad \rho_1(\mu) \sim \frac{7\mu^2}{60} - \frac{601\mu^4}{6300} + \frac{33\mu^6}{875} + O(\mu^8).
$$

Thus the correction terms are small for small amplitude breathers, and the frequency ($\omega$) requires less correction than the width.

Another point to note from the graphs is that when the width parameter is fixed (i.e. $\rho$ is exactly equal to $\Gamma \sin \nu$) and the frequency ($\omega$) and maximum amplitude ($\phi_0 = 4\mu$) are considered as perturbations then much larger corrections are found. Asymptotically we do this by introducing the new parameter $\nu$ in place of $\mu$, defined by $\mu = \nu - \Gamma^2 \rho_1(\nu) \tan \nu$. The effect of this is to alter the form of the perturbations to the other parameters as follows:

$$
\begin{align*}
\rho(\nu) &= \Gamma \sin \nu \left[ 1 + O(\Gamma^4) \right], \\
\phi_0(\nu) &= 4\nu \left[ 1 - \Gamma^2 \rho_1(\nu) \tan(\nu)/4\nu + O(\Gamma^4) \right] \\
&= 4\nu \left[ 1 + \Gamma^2 \varphi_{(n,1)}(\nu) + O(\Gamma^4) \right], \\
\omega(\nu) &= \Gamma \cos \nu \left[ 1 + \Gamma^2 \omega_1(\nu) + \Gamma^2 \rho_1(\nu) \tan^2 \nu + O(\Gamma^4) \right] \\
&= \Gamma \cos \nu \left[ 1 + \Gamma^2 \omega_{(n,1)}(\nu) + O(\Gamma^4) \right].
\end{align*}
$$

The fact that this produces much larger corrections we interpret as being due to the DSG breather not liking the shape being $1/\cosh(\cdots)$. Thus the major correction needed if a lossless mode exists is to the shape of the breather. This agrees with numerical calculations (spectral approximations calculated by Feddersen [1]), which show that the temporal behaviour of the breather in DSG is very close to SG results, but the spatial form needs more Fourier terms to gain a desirable accuracy.

These calculations can be carried out with any one of three parameters ($\omega, \rho, \phi_0$) fixed, and the discreteness effects represented as perturbations to the other two parameters. In the final form we fix $\omega = \Gamma \cos \eta$; for asymptotically small $\mu$ this is done by defining $\mu = \eta + \Gamma^2 \omega_1(\eta) \cot \eta$, then

$$
\begin{align*}
\rho &= \Gamma \sin \eta \left[ 1 + \Gamma^2 \rho_1(\eta) + \Gamma^2 \omega_1(\eta) \cot^2 \eta + O(\Gamma^4) \right] \\
&= \Gamma \sin \eta \left[ 1 + \Gamma^2 \varphi_{(n,1)}(\eta) + O(\Gamma^4) \right], \\
\phi_0 &= 4\eta \left[ 1 + \Gamma^2 \omega_1(\eta) \cot \eta/4\eta + O(\Gamma^4) \right] \\
&= 4\eta \left[ 1 + \Gamma^2 \varphi_{(n,1)}(\eta) + O(\Gamma^4) \right].
\end{align*}
$$

These three ways of viewing the correcting terms are entirely consistent with each other and agree with known results. These correcting terms are displayed in Fig. 2. Note that the corrections are much larger when plotted against $\nu$ than those against other parameters; showing that the shape requires greater modification than frequency of amplitude.

2.1. Energy of breather

It has already been mentioned that $H = T + U + \Gamma^2 V - W$ is not the energy of the breather, due to earlier rescalings. We should also note that since the approximation we have proposed is not an exact solution of the differential equations, the energy might vary slightly over the period of oscillation. To overcome this, we calculate the energy $E$ as an average over the time of one complete oscillation $(2\pi/\omega)$. 

We are now in a position to predict the energy of a DSG breather, and account for the differences introduced by discreteness. Combining the correcting terms we find

$$ E \sim 16 \Gamma \sin \mu \{ 1 + \Gamma^2 \mu \cot \mu \{ \omega_1(\mu) - \rho_1(\mu) \} - \frac{1}{288} \Gamma^2 (3 \mu \cot \mu - 3 + \sin^2 \mu + 6 \sin^4 \mu) \}. \quad (2.18) $$

Thus discreteness causes a reduction in the energy held by a breather of any given amplitude. Intuitively we expect the higher frequency to increase the energy of the breather, and the reduced width to lower the energy; our calculations show that this latter effect is larger and dominates the former. If we look at the expansion for small $\mu$, we see that the energy has an $O(\mu^2)$ correction

$$ E_1(\mu) \sim -\frac{7 \mu^2}{60} + \frac{47 \mu^4}{350} - \frac{1541 \mu^6}{23625}. \quad (2.19) $$
The correction $E_1(\mu)$ is plotted against $\mu$ in Fig. 3. This shows in more detail the reduction of energy for small amplitude breathers, and the turning point at $\mu \approx 0.85$, where the relative energy difference is maximal.

3. Concluding remarks

The method used in this paper relies on the knowledge of the continuum SG breather. It does not rely on the integrability of the SG system. It uses the known SG breather as a basis for an asymptotic expansion in the discreteness parameter. The use of Hamilton’s Principal and the Calculus of Variations gives a strong theoretical basis to the method, and we thus have considerable confidence in the predictions made by this method.

Our results support the numerical work, showing that for small amplitude breathers the effects of discreteness are also small. However for larger amplitude, the effects grow, and could cause losses to the mode. In the limit where the SG breather would be splitting into two counter-propagating kinks, the results presented here show that large corrections are needed to the shape and evolution of the DSG system. This method cannot account for what might happen in this case.

The method predicts corrections to the SG frequency–amplitude relationship caused by discreteness. It also accounts for the spatial form of the breather requiring greater correction than the temporal evolution. This is also observed in numerical work [1,14] in that many more spatial Fourier modes than temporal modes are needed to gain reasonable accuracy. But unlike an earlier paper [10] it does not give a detailed prescription of how the shape needs to be corrected.

We can also find the corresponding corrections to the energy that are caused by discreteness. Some of these corrections are direct, others through the fact that discreteness causes an increase in the frequency of the breather and a reduction in the width of the breather; i.e. the breather extends over fewer lattice sites than the purely continuum SG theory predicts, for a breather of similar maximum amplitude.

References