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Bifurcation of Internal Solitary Wave Modes from the Essential Spectrum

by

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ABSTRACT

The bifurcation of internal modes from the phonon band in models supporting solitary wave solutions has been one of the exciting new phenomena in the field. We will present a number of analytical and semi-analytical techniques for the detection, study and understanding of these modes. We will see how they appear, without threshold, due to the discretization of the continuum equations. This perturbation is viewed in terms of a singular continuum approximation and analyzed by both perturbation theory and the Evans' function method. It is shown that these methods give equivalent results. Moreover, they are corroborated by mixed analytical-numerical computations based on the discrete Evans' function recently developed by the first author. The extent to which these predictions survive to strong discretizations are discussed. The results will be presented in the context of both the sine-Gordon and the ϕ^4 models.

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1 Introduction

In the past few decades, solitary wave solutions have been recognized as a characteristic of many physical systems ranging from information transmission in Josephson junctions and optical fiber arrays ([1]-[5]) to the transcription of genetic material and the local denaturation of the base pair hydrogen bonds in the DNA double helix ([6]-[10]). It has been recognized, however, that many of these applications (such as the Josephson junctions, the DNA problem, the motion of dislocations in solid state physics [11]-[13], or even the behavior of an array of coupled torsion pendula, [14]) are inherently discrete in nature and thus necessitate that the problem be studied in the context of a lattice. Hence in the past two decades there has been a rapidly increasing number of papers that are concerned with the drastic modifications of the continuum solitary wave system behavior, once it is posed on a lattice. The first very important contribution in identifying these traits was given by Peyrard and Kruskal, [15], and also in the more recent papers of Combs and Yip, [16], as well as Ishimori and Munakata, [17].

In brief, the main changes that occur when studying models with Hamiltonian structure supporting solitary wave solutions as a discrete system are the following:

- The breaking of translational invariance creates a non-zero Goldstone frequency which coupled to the phonons creates wave excitations radiating energy away from the coherent structure and, thus, contributing to its energy loss.

- Also, all the configurations are no longer equivalent on the lattice but there is a max energy (kink centered on a site) and a minimum energy (kink centered between sites) configuration leading to the creation of a barrier analogous to the one dislocations have to overcome in order to propagate on a lattice and hence termed the Peierls-Nabarro (P-N) barrier.

- Due to the resonances, the gradual kinetic energy loss leads to pinning (trapping) in one of the P-N barriers between two lattice sites and the resonance of the oscillation frequency therein finally drives the kink to become static relaxing in the stable steady state.

However, even though there was a series of papers that elaborated on and clarified the above issues (i.e. the resonances [18]-[19], the P-N oscillation [20]-[19], the stability of coherent soliton-like structures on diffusively coupled lattices [21] as well as the collective variable behavior of these structures [22]-[26]), not all of the story was unveiled. In particular, Braun, Peyrard and Kivshar observed much later ([27]) that in a range of parameter values for the discrete sine Gordon equation (also known as the Frenkel-Kontorova model and originally proposed for the study of dislocations, [11]) that a discrete mode bifurcated from the bottom edge of the phonon spectrum. Both mathematically and physically the study of this bifurcation is an important problem:

- Mathematically, because one can develop techniques to quantitatively predict when this bifurcation will occur and what its magnitude will be;

- and physically because this internal mode will create oscillations that will modify the shape of the transmitted information (i.e. in the array of coupled Josephson junctions) and one would be interested in finding out what the form will be of this shaping factor (and thus its effect on the transmitted bits/kinks) and the regime where it will appear.

One important subsequent paper of Kivshar et al. ([28]) revealed the characteristic that the birth of these internal modes is thresholdless (i.e., appears as soon as the continuum problem is set on a lattice). It also gave a quantitative method of prediction of the magnitude of these bifurcations based on singular perturbation theory.

Our aim in this paper will be two-fold:

1. For two important models that support soliton-like solutions, namely the discrete sine-Gordon and the ϕ^4 model, we will first study discreteness as a perturbation of the continuum through the singular perturbation theory proposed in [28] and through the Evans function as proposed in [29]-[30]. We will show the equivalence of the two approaches for this problem and will quantify their predictions.

2. On the other hand, using linear stability analysis and a semi-analytical methodology, introduced in [21], the discrete Evans function technique, we will trace the exact perturbation of the discrete internal mode from the phonon band and will indicate where (and why) the continuum method fails.

In this way, we hope to provide a comprehensive set of tools and of results pertinent to this problem in order to reveal the main characteristics and the physical aspects of the behavior of these solitary wave modes.

Our presentation will be organized as follows: In section 2 we will follow the approach of [28] in presenting the singular perturbation methodology. In section 3, the continuum Evans function approach will be presented and the equivalence of its results to the results in section 2 will be established. In section 4, the discrete Evans technique will be introduced and implemented. Its results will be compared to linear stability analysis and to the continuum perturbation methods. Finally, in section 5, a summary of the results and conclusions as well as an outlook of potential extensions of this work will be outlined.

2 Perturbation Theory

Let us consider the case of the sine-Gordon equation treating discreteness as a perturbation. Following the notation of [28] we can write it as:

$$u_{tt} = u_{xx} - \sin u + \epsilon g(u)$$

where $\epsilon = \frac{h^2}{12}$ and $g(u) = u_{xxxx}$ if we consider only the 4th. derivative (i.e. the first order perturbation in the expansion: $\frac{u_{i+1}+u_{i-1}-2u_i}{h^2} = \sum \frac{2h^{2j}}{2j!}\frac{\partial^{2j}u}{\partial x^{2j}}$).

The expression of the perturbation can be suitably modified if higher order terms are included. Expressing the solution as a perturbation series, as well, $u = u^0 + \epsilon u^1$ one can explicitly derive the equation for u^1 to be

$$u^1_{xx} - \cos u^0 u^1 = g(u^0)$$

and can find the solution to be:

$$u^1(x) = \frac{1}{\cosh x}\int_{-\infty}^{x} dx' \cosh^2 x' \int_{-\infty}^{x'} dx'' \frac{g(u^0)}{\cosh x''}$$

It is important here to make the observation that the lower limit of our integration is $-\infty$ as opposed to 0 as appears in [28]. For the case of the sine Gordon with 4th. and/or higher order derivative perturbation explicit calculation can show that the integral with zero lower bound yields a divergence (as the astute reader can readily realize viewing the lower bound of the innermost integral's integrand as a constant and seeing the divergence arise from $\frac{1}{\cosh x}\int^x dx' \cosh^2 x'$) Thus, this substitution is necessary in order to avoid any unphysical divergences. In order to construct the spectrum around this perturbed solution one expands in linearized excitations around the kink solution $u(x,t) = u^0 + \epsilon u^1 + w(x)\exp(i\omega t) +$. The linearized equation for the perturbed eigenfunctions is then:

$$-\omega^2 w = w_{xx} + (\frac{2}{\cosh^2 x} - 1)w + \epsilon u^1 \sin u^0$$

Remembering that the unperturbed eigenfunctions of the continuum fully integrable sine-Gordon model are ([31]) :$W(x,k) = \exp(ikx)\frac{k+i\tanh x}{k+i}$ for a continuum of wavenumbers satisfying the linear dispersion relation $\omega^2 = 1 + k^2$ -the band edge ($k = 0$) of which grows secularly (as a $\tanh x$), we can expand the perturbed linearized excitations in the basis of the unperturbed ones. The equation for the coefficients of this basis expansion is then:

$$a(k) = \frac{\epsilon}{2\pi}\int_{-\infty}^{\infty} \frac{K(k,k')a(k')dk'}{k'^2 + \epsilon^2 b^2}$$

where $K =< W|f|W >$ is a Fourier space integral kernel and the bifurcating eigenvalue has a frequency ${\omega_b}^2 = 1 - \epsilon^2 b^2$. The authors of [28] extracted the singular contribution to the integral by setting $k' = 0$ in the numerator and integrating over the Lorentzian curve. The demand of self-consistency then yields an equation for the value of the bifurcation parameter b:

$$|b| = \frac{1}{2} sgn(\epsilon) \int_{-\infty}^{\infty} \tanh x^2 u^1 \sin u^0 dx$$

Up to now, we have, briefly, reproduced the arguments given in [28]. Even though some of the details may be deemed as unnecessary as the full presentation is given in [28], we believe that in view of the establishment of the equivalence of the results of the method with the continuum Evans function technique, as well as for reasons of general reference and methodology, their presentation is useful. For the case of the sine-Gordon, we have studied not only the case of quartic but also of 6th. and higher order perturbations and we give the full results below. In the case of the quartic, the functional form of u^1 can be explicitly found to be:

$$u^1(x) = (-3 + \frac{6 + x + \exp(2x)x}{(1 + \exp(2x))}) / \cosh x$$

We will give the parametric dependence of the results for both models in accordance with their form as it appears in the standard reference in the subject ([15]). The discrete lattice equations of the Frenkel Kontorova model are then:

$$u_{tt} = u_{i+1} + u_{i-1} - 2u_i - \frac{1}{d^2} \sin u_i$$

and using the appropriate rescaling $h \rightarrow 1/d$, $\omega \rightarrow d\omega$ the bifurcation parameter of the discrete mode will be (up to 2nd. order perturbative corrections) :

$$\epsilon b = \frac{1}{2} (\frac{0.08888889}{d^2} - \frac{0.0047619}{d^4})$$

Higher orders can be seen to saturate to this order of correction to a very good degree of approximation. The discrete mode then detaching from the bottom edge

($\omega = 1/d$) of the phonon band will have a frequency $\omega = \frac{1}{d^2}(1 - \epsilon^2 b^2)$. On the other hand similarly the discrete ϕ^4 assumes the form:

$$u_{tt} = u_{i+1} + u_{i-1} - 2u_i + \frac{1}{d^2}(u_i - u_i^3)$$

and again by using the appropriate rescaling, $h^2 \to 1/(2d^2)$, $\omega \to \sqrt{2}d\omega$, of the notation of [28] one can find that the bifurcating frequency will be:

$$\omega^2 = \frac{2}{d^2} - \frac{2}{15^2 d^6}$$

away from the bottom edge ($\sqrt{2}/d$) of the essential spectrum (to first order which as claimed in [28] gives an excellent approximation to the numerical predictions. The accuracy of this statement will be examined later). We have, so far, reformulated (making some minor modifications) and presented the methodology of [27]-[28] in identifying and quantifying the bifurcation of discrete modes from the bottom edge of the essential spectrum and we have also applied this methodology to the discrete sine Gordon and ϕ^4 model. Let us now present an alternative approach as given in the context of the perturbed nonlinear Schrödinger equation in [29]-[30] that will complement this presentation yielding an equivalent formulation.

3 Continuum Evans Function

First, we give the basic idea behind the Evans function method. If one writes down an eigenvalue problem, such as the unperturbed or the perturbed ones presented above, then there are eigenvalue solutions with positive as well as ones with negative real part. If one finds the span of the invariant subspace associated with all the eigenvalues of positive real part, then one obtains the unstable manifold of solutions decaying exponentially backward in time E^u. On the other hand, tracing the negative real part ones, their span yields the stable manifold, that decays exponentially forward in time, E^s. If the two intersect i.e. their wedge product, defined to be the Evans function: $E(\omega) = E^u \wedge E^s$, has a frequency for which it is zero then, by construction, it is an eigenvalue (as there is an associated solution decaying exponentially in both time directions). Thus, the Evans function is a function whose zeros yield the discrete modes pertaining to the coherent structure sustained by the model under study. Coming back to our example, the eigenvalue problem can be written (using notation in accordance to [29]) as :

$$Y' = M(x, \omega, \epsilon)Y$$

where the matrix M is:

$$M = \begin{bmatrix} 0 & 1 \\ g(x) - \omega^2 & 0 \end{bmatrix}$$

and $g(x) = 1 - \frac{2}{\cosh^2 x} - \epsilon u^1 \sin u^0$ as can be seen from the previous section. Setting

$$M_0 = \lim_{|x| \to \infty} M(\omega, x, 0)$$

the eigenvalues of this limit matrix are $\pm\gamma$ where $\gamma = -ik = \sqrt{|\omega^2 - 1|}\exp(\frac{i}{2}\arg(1 - \omega^2))$ for $\arg(1-\omega^2) \in [-\frac{\pi}{2}, \frac{3\pi}{2})$ (the details of why we consider the branch cuts can be found in [29] but will also be clear later on in this presentation). The corresponding eigenfunctions are $[1, \pm\gamma]$.

In our case, however, ([31],[28]) we also know (both in the case of the SG as well as in the ϕ^4 the full scattering operator eigenspectrum and the corresponding set of eigenfunctions. In the SG case the forward time decaying eigenfunctions will be :

$$Y^+ = \begin{bmatrix} P(\gamma, x) \\ Q(\gamma, x) \end{bmatrix}$$

where $P(\gamma, x) = \exp(-\gamma x)\frac{\gamma+\tanh x}{\gamma+1}$ and $Q = P'$. On the other hand the solutions exponentially decaying backward in time are :

$$Y^- = \begin{bmatrix} P(\gamma, -x) \\ -Q(\gamma, -x) \end{bmatrix}$$

where P, Q again as defined above. Furthermore, it is straightforward to verify that the adjoint problem $Z' = -M^T Z$ has as solutions (that will be used in what follows): $Z = [-Q(\omega, x), P(\omega, x)]^T$ One can verify the following limit relations (analogous to (3.5) of [29]):

$$\lim_{x \to \mp\infty} Y^- \exp(\mp\gamma x) = [1, \pm\gamma]^T$$

and

$$\lim_{x\to\pm\infty} Y^- \exp(\mp\gamma x) = \frac{\gamma-1}{\gamma+1}[1, \pm\gamma]^T$$

Then, using the above definition of the Evans function: $E(\omega) = Y^- \wedge Y^+$ one finds:

$$E = 2\gamma(1 - \frac{2\gamma}{1+\gamma})$$

that can be written as (see remark 4.3, [29]) :

$$E = 2\gamma(1 + g_2(\omega))$$

with g_2 continuous and vanishing at the bottom edge of the phonon band. On the other hand according to Theorem 4.2 of [29] the derivative of the Evans function evaluated at the bottom edge of the phonon band is:

$$\partial E_\epsilon(1/d, \epsilon = 0) = \int_{-\infty}^{\infty} Z(1/d, x, 0)\partial M_\epsilon(1/d, x, 0)Y^+(1/d, x, 0)dx$$

(where as usual the subscript denotes partial derivative with respect to the subscript variable) In the sine-Gordon case :

$$\partial E_\epsilon(1/d, \epsilon = 0) = -\int_{-\infty}^{\infty} \tanh^2 x u^1 sin(u^0)dx$$

an expression which is certainly familiar from the presentation in the previous section. Now using the differentiability of the Evans function to expand it in a Taylor series around the bottom edge of the essential spectrum we get : $E(\omega, \epsilon) = E(\omega, 0) + (\partial E_\epsilon(1/d, \epsilon = 0) + g_1(\omega, \epsilon))\epsilon$ where g_1 is also continuous and vanishing at $\omega = 1/d$. Then, if the argument of the derivative does not belong in the domain $(-\frac{\pi}{4}, \frac{3\pi}{4})$ (due to the branch cuts taken above), then there is no bifurcation. In our case this statement translates to: $sign(\epsilon)\int_{-\infty}^{\infty}\tanh^2(x)u^1\sin(u^0)dx$ being negative. But in that case, also, the absolute value of b as defined in the previous section according to [28] would be negative and thus no bifurcation would occur. On the other hand if the quantity above is positive then the vanishing of $E(\omega,\epsilon)$ will occur according to the expansion at $\omega^2=\frac{1}{d^2}(1-\epsilon^2b^2)$ where b is defined exactly as in the perturbation theory treatment. Hence the two approaches are shown to yield the exact same result for the bifurcation of the discrete mode from the bottom edge of the continuum spectrum of the sine-Gordon equation. Furthermore, since the condition is satisfied for the appearance of the mode (as the predictions made in the previous section indicate) for any d, the discrete mode should (according to these predictions) be present for all d as soon as one studies the problem on the lattice (hence, its generation is threshold-less). The proof is exactly the same in the case of the ϕ^4 model and will be left to the reader, as an interesting exercise. The only thing that changes is the form of the unperturbed spectrum and the form of the perturbation that is dependent on the non-linearity. Otherwise, the verification of the equivalence of the two methods can follow the exact same path.

It is perhaps not surprising that the two methods render the same answer. The derivative of the Evans function is known to be equivalent to a Melnikov function, see [35]. It is also well-known that Melnikov calculations can be derived in alternative way using a solvability condition, see [36]. The singular perturbation theory approach used above fits into this framework and thus the equivalence of the results coming from the two methods is based on the equivalence of the two methods as the two different approaches to the Melnikov method.

Having presented the two approaches that treat discreteness as a perturbation, we will now give a semi-analytical method which corresponds to the discrete version of the Evans function technique and which first appeared in [21], Its results will subsequently be compared with those of the above methods and with the ones from linear stability analysis and the differences will be highlighted and explained.

4 Semi-Analytical Methods and Comparison

Let us revisit the lattice problem, reconsidering the idea behind the construction of the Evans function (in presenting it we will also give the details of performing linear stability analysis computations, as some of them will be pertinent to the construction of the discrete Evans function). In order to construct a discrete eigenfunction one must find a solution that decays to the left as well as to the right far away from the coherent structure. However, the kink decays, in the sine Gordon equation, to the left exponentially to 0 and to the right to 2π whereas in the ϕ^4 the corresponding decay is to -1 to the left and 1 to the right.The linearized equation around the coherent structure will read:

$$\omega^2 u_i = u_{i+1} + u_{i-1} - 2u_i - \frac{1}{d^2}\cos K_i u_i$$

in the SG and

$$\omega^2 u_i = u_{i+1} + u_{i-1} - 2u_i - \frac{1}{d^2}(3{K_i}^2 - 1)u_i$$

in ϕ^4.

In order to trace the discrete eigenvalues, the most simple numerical method is to solve the full eigenvalue problem presented through the above equations as follows:

- Cosntruct the exact discrete kink, through a Newton-Raphson iteration solving the system of equations:

$$y_{i+1} + y_{i-1} - 2y_i - \frac{1}{d^2} \sin y_i = 0$$

  (analogously defined for ϕ^4) with a continuum kink initial condition.

- Using the exact discrete kink K, as constructed above, one can solve the discrete eigenvalue problem to track down both the discrete frequencies as well as the linear extended phonon excitations (and their eigenfunctions).

On the other hand, if one is after only the discrete modes, one has to construct a decaying solution far away from the kink, on either side of the lattice. The linearized equation is simplified far away from the kink as $\cos K_i \to 1$ and $3{K_i}^2 - 1 \to 2$. Thus one obtains a second order difference equation whose solutions are of the form:

$$u_i = C_\pm(\omega){r_1}^i + D_\pm(\omega){r_2}^i$$

with:

$$r_{2,1} = \frac{1}{2}[\omega^2 + 2 + \frac{1}{d^2} \pm \sqrt{(\omega^2 + \frac{1}{d^2})(\omega^2 + \frac{1}{d^2} + 4)}]$$

for the SG and $\frac{1}{d^2} \to \frac{2}{d^2}$ for the ϕ^4 (we will, hereafter, present the construction for the SG with the understanding the the ϕ^4 construction will entail only this minor difference which can be readily observed to correspond to the difference in the phonon band edge).

Then if one starts off to the left of the kink with $u_i = D_- {r_2}^i$ (which has the right exponential decay behavior) and shoots through the coherent structure, one is going to pick, on the right side, a solution with both decaying and growing parts ie.:

$$u_i = C_+ {r_1}^i + D_+ {r_2}^i$$

where now D_+ pertains to the growing part. Hence if one finds a frequency that annihilates the prefactor of the growing part, D_+, then one is left with a solution that decays on both sides of the coherent structure and is thus an eigenfunction. The continuation of the iteration to $i = L$ and assuming the above equation for the u_i on the right of the kink as holding for the sites $L-1, L, L+1$ of the lattice (which is a statement with exponentially small corrections away from the kink), then

$$D_+ = \frac{u_{L+1} - r_1 u_L}{{r_2}^{L+1} - {r_2}^L r_1} = \frac{r_2 u_L - u_{L-1}}{{r_2}^{L-1}({r_2}^2 - 1)}$$

For the technical (normalization) reasons explained in [21], we start off on the left side with $D_- = {r_1}^{2L}$ (where L is the size of our lattice) and also we remove the branch cuts introduced from the edges of the phonon band (${r_2}^2 = 1$) in the above equation, by appropriately rescaling (see [21]).

Having setup all the methods relevant to the problem of the study of the internal shape mode bifurcations from the essential spectrum we will now present their results for the two discrete models of concern to this study. Linear stability analysis shows that:

- In the sine-Gordon model, (fig. [1]), the spectrum consists of a discrete Goldstone mode that, due to the breaking of the translational invariance has a non-zero frequency (that will resonate with the phonons as established in [19]-[20]), and a phonon band in the frequency range of $[\frac{1}{d}, \sqrt{4+\frac{1}{d^2}}]$ (as can be seen from the linear dispersion relation $\omega^2 = 2 - 2\cos k + \frac{1}{d^2}$). In addition, after $d \approx 0.515$ a shape mode bifurcates from the bottom of the phonon band. Its maximum frequency bifurcation from the $1/d$ of the essential spectrum bottom edge can be seen to occur around $d = 0.7$ and then the spatial form of the eigenfunction appears to change sign and the bifurcation distance to decrease until $d \approx 1.3$. Thereafter the mode sits almost at the edge of the band (a distance of the order of 10^{-5} or less away and even though it maintains its parity parity, it, now, gradually degenerates to extend over the whole lattice. For larger lattices, this occurs for larger d and for the infinite lattice (presumably) the degeneration occurs for $d \approx \infty$ justifying the conclusion of the thresholdless birth of the solitary wave discrete shape eigenmode.

- In the ϕ^4 case, the spectrum, (fig. [2]), has always at least 2 kink eigenmodes ie. not only the Goldstone mode (which in this case, also, bifurcates from zero) but also the second mode corresponding to its continuum sibling with frequency $\sqrt{\frac{3}{2d^2}}$. The phonon band lies between $[\frac{\sqrt{2}}{d}, \sqrt{4+\frac{2}{d^2}}]$. The internal kink mode that bifurcates from the bottom edge of the band appears for d close to 0.81, maximizes its distance from it at $d \approx 1.05$ and changes its sign and thereafter approaches again $\frac{2}{d}$ in a similar manner to the one described above.

The results for the internal mode bifurcation (indicated by $\star$ in figures [3],[4] for the two models) coincide exactly (with the exception of only slight deviations of the order of 10^{-5}, that cannot be discerned in figs. [3]-[4] for the 400 site lattice has been used in the numerical experiments, for large d's due to the finite size effect outlined previously, see ie. fig. [4] of [21]) with the ones from linear stability analysis. Thus the discrete Evans technique is one that can very accurately identify the discrete modes and their bifurcation from the essential spectrum. The Evans function results have been constructed using a secant iteration to identify the zeros of the Evans function along the imaginary spectral plane axis (where the shape mode eigenfrequency has to lie, due to the Hamiltonian nature of the system). Moreover the Evans function value at the bottom of the band edge can be used as a diagnostic, according to [21], as it was observed there that the change of sign from negative to positive indicates the detachment of the internal mode from the edge. However, considering the fact that the unperturbed continuum Evans function vanishes at the bottom edge of the essential spectrum and the $\epsilon\partial E_\epsilon$ sign change which indicates the bifurcation (according to the criterion of [29]-[30] and/or equivalently (as we proved) of [27]-[28]), and also taking into consideration the rescaling sign change when multiplying the discrete Evans function by $\frac{{r_2}^2-1}{{r_2}^2}$, the discrete Evans function criterion postulated in [21] is equivalent to the ones of [27]-[30] ! On the other hand, viewing the predictions of the continuum theories that treat discreteness as a perturbation (indicated by solid lines in figs. [3]-[4]) we realize that their predictions are quite successful close to the continuum limit (ie. for large d). As $d \downarrow$, however, their prediction is close to the results of the (close to exact) semi-analytical/numerical methods down to $d \approx 0.9$ in the SG and 1.2 in the ϕ^4 case. For lower values of the discreteness parameter (for strong discreteness) the perturbative treatments fail quite dramatically. Of course, it is well known from previous attempts to treat discreteness as a perturbation (see, for instance, [17] where the singular perturbation treatment of Keener-McLaughlin, McLaughlin-Scott ([32]-[33]) was implemented to treat discreteness), that such methods cannot account for the drastic implications of discreteness for lattices in which the atoms are far apart. Hence, such a radical difference between the blowing up (for $d \rightarrow 0$) prediction of the continuum theories and the smooth behavior of the internal wave mode that is of the same parity as the second (in SG) and the third (in ϕ^4) derivative of the kink, is to be anticipated. However, one can go a step further to explain why this type of qualitative behavior (i.e., reaching a maximal bifurcation and then smoothly going to 0 for finite d) is to be expected as $d \rightarrow 0$. In particular, as d decreases, the explicit Newton-Raphson of the kink site ordinates, shows that fewer of them participate in the "spine" of the kink (which is in accordance also with what one expects in the continuum theory where the width of the spine is explicitly known, see ie. [34]). For example in the SG, for $d < 1$, practically only 6 sites contribute to the kink structure with ordinates symmetrically (the first and the sixth, the second and the fifth etc.) adding up to 2π. In addition, only one of the 3 ordinates $< \pi$ is $> \frac{\pi}{2}$. That site falls below $\pi/2$ after $d = 0.7$. This can be very accurately also predicted by the 6 point-kink approximate equations for a kink of the approximate structure $(0, ..., 0, a, b, c, 2\pi - c, 2\pi - b, 2\pi - a, 2\pi, ..., 2\pi)$. These equations read:

$$b - 2a - \frac{1}{d^2} \sin a = 0$$

$$c + a - 2b - \frac{1}{d^2} \sin b = 0$$

$$b + 2\pi - 3c - \frac{1}{d^2} \sin c = 0$$

and predict a solution with $c < \pi/2$ for $d < 0.707$. When this occurs, the sign of $\cos c$ in the linearized equations:

$$y_{i+1} + y_{i-1} - 2y_i - \frac{1}{d^2}\cos K_i y_i = -\omega^2 y_i$$

will change (and practically all other cosine terms will be ≈ 1) and thus in order to maintain the functional form and parity of the mode the solution changes sign $y_i \to -y_i$ as the linear stability analysis verifies. As d decreases further, only four and then two sites contribute to the kink (ie. for $d = 0.3$ the kink is practically a two site kink and the only sites contributing to its spine have $\cos a = \cos 2\pi - a \approx 0.9$). Thus the linearized equation approaches (for gradually decreasing d) the one with $\cos K_i = 1$, hence giving birth not to discrete coherent structure eigenmodes but to linearized extended phonon excitations around the uniform steady states. The limit of $d = 0$ will, of course, find all sites to the left of the kink at the $u = 0$ steady state whereas to the right at $u = 2\pi$ (the equivalent picture in ϕ^4 is straightforward to draw). Hence, it is due to the fact that the kink on the lattice consists of few sites with ordinates differing from the uniform steady state ones, that causes the internal mode to bifurcate maximally and then to change its spatial profile sign and gradually degenerate for sufficiently small d to an extended excitation and thus disappear in strict conflict with the continuum theory prediction. The continuum theories, treating discreteness as a continuum-like perturbation miss this essential trait and always see the kink as a translationally invariant structure that with a spine that consists of infinite points. This prevents their prediction from realizing that as the lattice becomes more and more discrete the kink is less and less densely populated until in the end the linearized equation matches the one of the continuum eigenmodes that satisfy the linear wave dispersion relation. This argument, we believe, highlights the point of difference between the semi-analytical or numerical techniques and the continuum-like theoretical predictions and indicates what needs to be refined in order for these theories to be able to capture the features of the strong discreteness regime.

Let us, now, summarize the results of this presentation in the following (and last) section.

5 Conclusions & Future Challenges

The scope of this paper has been three-fold:

1. First, to present the continuum methods, such as perturbative treatments or the continuum Evans function technique that approach the problem of the internal mode bifurcation viewing discreteness as a perturbation and to demonstrate the equivalence of results of these techniques.

2. Secondly, to indicate the semi-analytical or numerical methods that one can use in order to perform numerical experiments identifying these modes and the magnitude of the bifurcation from the bottom edge of the essential spectrum. Linear stability analysis and the discrete Evans function were used in that direction and the near identity of their (numerical) results was demonstrated.

3. Finally the continuum-like methods were compared to the numerical results and the regimes of the coincidence of their prediction with the numerical experiment were indicated. Also highlighted was the failure of these techniques to capture the regime of high discreteness as well as the reason for it (the sparsely populated spine of the discrete kink-like structure). In that context the qualitative picture of the internal mode behavior as produced by the numerical simulations was justified by means of simple physical arguments.

We have, thus, used a combination of available techniques and tools to study in the two models of interest, the SG and ϕ^4 discrete model equations, the

thresholdless generation of an internal mode pertaining to the kink solitary wave (and corresponding in parity to one of its spatial derivatives) due to the perturbing discreteness. The smooth maximization of the bifurcation and the vanishing of the mode for strongly discrete lattices were numerically indicated and the disparity of this prediction from its blowing up according to the perturbative methodologies clarified.

An interesting extension of this study would involve an attempt to create a rigorous perturbative technique that could, possibly, study theoretically and predict, in good agreement with the numerical findings, the mode frequency behavior in the highly discrete (small d) versions of the lattice models. This challenging theoretical task will be left for future studies.

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Figure Captions

Fig. 1: Spectrum of Sine Gordon Equation for d=0.7.Upper Left: Full Spectrum, Upper Right: Goldstone Mode, Down Left: Internal Shape Mode, Down Right: Coherent Structure and Phonon Band frequencies' Parametric Dependence (vs. d) -Results from Linear Stability Analysis-.

Fig. 2: Spectrum of ϕ^4 for d=1.0.Upper Left: Goldstone Mode, Upper Right: Second Discrete Mode, Down Left: Internal Mode, Down Right: Coherent Structure and Phonon Band frequencies' Parametric Dependence (vs. d) -Results from Linear Stability Analysis-.

Fig. 3: Bifurcation of Internal Mode in SG vs. the Discreteness Parameter

Fig. 4: Same as the Previous but for the ϕ^4 Model.

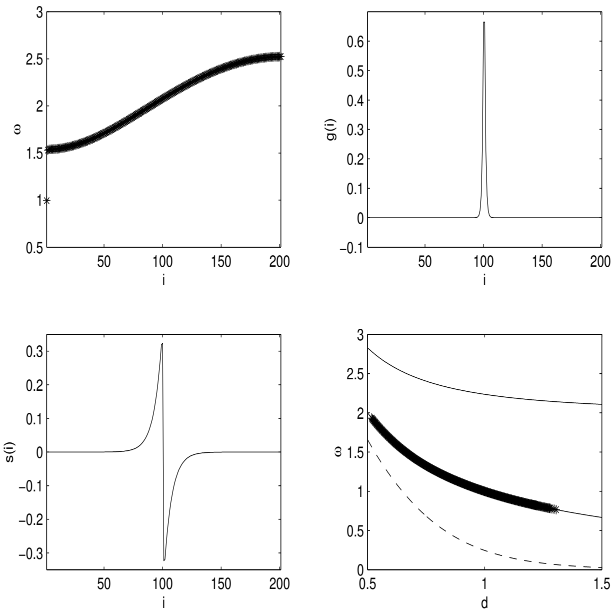


Figure 1

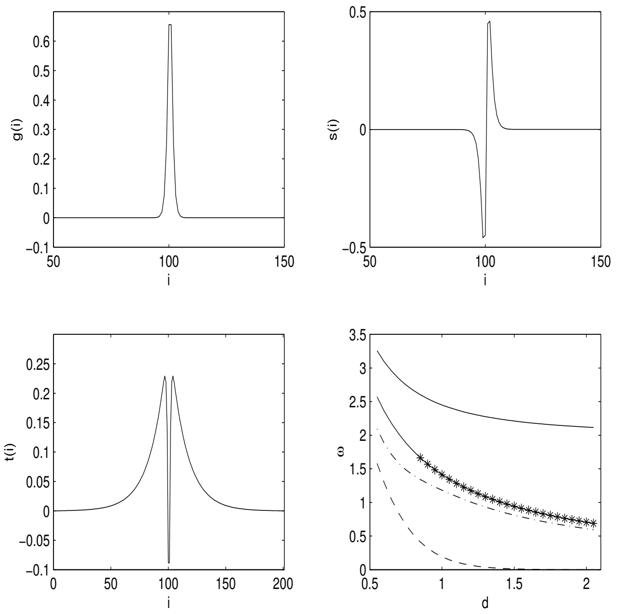
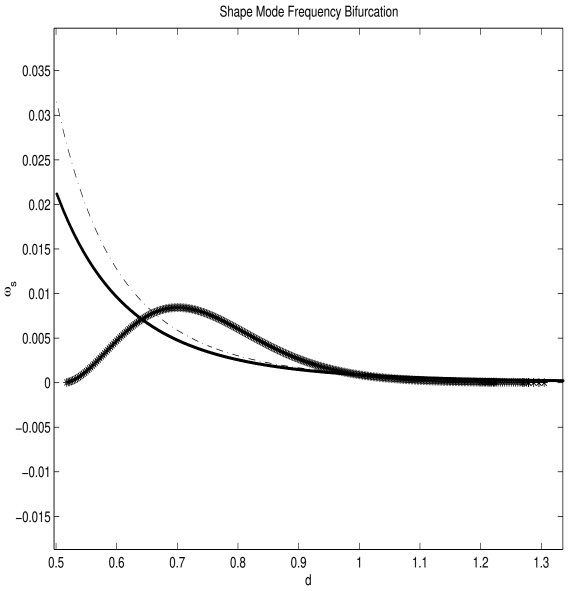


Figure 2


Shape Mode Frequency Bifurcation
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0.03
0.025
0.02
0.015
0.01
0.005
0
−0.005
−0.01
−0.015
ω_s
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
d

Figure 3

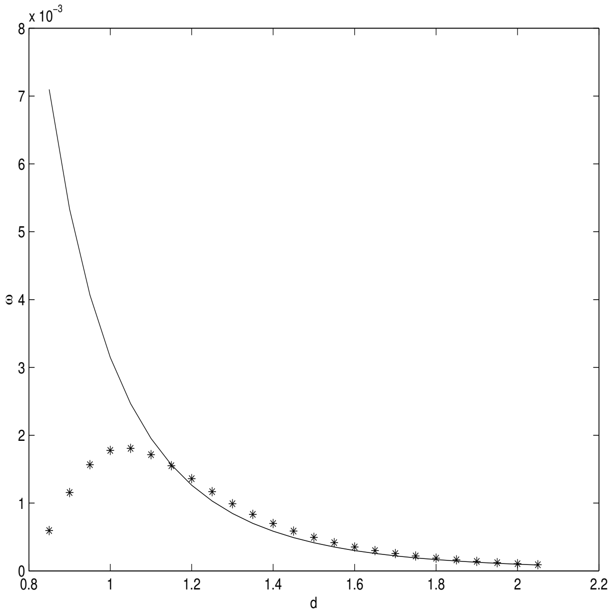

Figure 4