Soliton internal mode bifurcations: Pure power law?

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The bifurcation of internal solitary wave modes from the essential spectrum has been one of the most exciting recent developments in the study of soliton dynamics. To date, it was believed that the bifurcation of such modes due to discretization has a strict power law dependence on the lattice discreteness parameter. In this work we prove that this dependence actually possesses relevant exponentially small terms which distinguish between different solutions for the discrete models. The theoretical result is established by using a discrete version of the Evans function. The predictions presented herein compare very favorably with the numerical study of the linear eigenvalue problem, and offer explanations of computational effects not possible on the basis of previous theoretical studies.

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The ubiquity of solitary waves in physical applications [1] has triggered, over the past few decades, an intense theoretical and experimental effort to study and understand these nonlinear waves. Even though most of the initial attempts to study such phenomena were in the continuum setup of Hamiltonian nonlinear partial differential equations (see Refs. [1,2] for reviews of relevant problems and results), it was more recently realized that many of the relevant applications were inherently discrete. When considering the motion of dislocations in solid state physics [3], the local denaturation of the DNA double strand [4] (and references therein), arrays of Josephson junctions, and optical fibers for information transmission [5–7] (and references therein), to name a few, the relevant problems have to be studied on a lattice.

The study of such excitations on a lattice over the past two decades revealed a completely different picture than the one that was known for their continuum siblings. The breaking of translational invariance (TI) was found to generically produce two static steady states (one stable and one unstable) due to the corresponding bifurcation of the translational modes in the spectral plane [8–11]. In addition, edge modes were found to bifurcate from the phonon band and give rise to localized eigenmodes of the soliton [12–14]. The resonance of the harmonics of relevant eigenmodes (a finite-dimensional subspace) with the infinite-dimensional space of extended eigenmodes was found to give rise to nonlinear damping [15,16] that would brake and eventually trap the solitons.

In this paper, we will revisit one aspect of this picture, namely, the bifurcation of internal solitary wave modes from the phonon band. This aspect is particularly important since not only are these modes relevant to the radiation problem in identifying the resonance picture [15], but also because they may affect (modulate) the nature of the transmitted information. As identified in early numerical experiments [16,17], and proved in Ref. [15], such modes may create genuinely periodic asymptotic states in which one such mode has persistent oscillations of nonzero amplitude. One may think of such periodic solutions as breathers (since they are time periodic and exponentially localized in space) mounted on a kink background. Furthermore, preliminary results of recent work by one of the present authors [18] indicated that the presence of such internal modes may be directly related to the absence of integrability in such systems. Hence it is vital to have a physical and mathematical handle on the behavior of such objects.

These modes were observed for the first time in the discrete sine Gordon (SG) equation

$$u_{n,tt}=u_{n+1}+u_{n-1}-2u_n-\frac{1}{d^2}\sin u_n \tag{1}$$

[where $u(n,t)$ is the field, subscript n denotes the lattice site and subscript t the time derivative, and $d=1/\Delta x$ is the discreteness parameter, i.e., the inverse lattice spacing] by Braun, Kivshar and Peyard [12]. Subsequent theoretical work by Kivshar *et al.* [19] predicted that these modes would bifurcate by an amount $O(1/d^4)$ from the edge of the phonon band which lies at $1/d$ (the dispersion relation reads $\omega^2=-(1/d^2+2-2\cos k)$, hence permitting extended waves with frequencies in the interval $\pm i[1/d,\sqrt{4+1/d^2}]$). Their reasoning was based on the Taylor expansion

$$\frac{u_{n+1}+u_{n-1}-2u_n}{\Delta x^2}=\sum_{j=1}^{\infty}\frac{2\Delta x^{2j-2}}{2j!}\frac{d^{2j}u}{dx^{2j}}. \tag{2}$$

In particular, discreteness was treated as a singular fourth (leading) order derivative perturbation to the continuum problem. Using solvability conditions within perturbation theory, they were able to establish a bifurcation from the band edge of the form

$$\omega^2=\omega_{edge}^2(1-\epsilon^2 b^2), \tag{3}$$

where $\epsilon=\Delta x^2/12$ is the perturbation parameter and b the self-consistently determined (through the solvability conditions) detuning parameter [13,19]. Using the same strategy (discreteness as a leading order perturbation in the Taylor series) Kevrekidis and Jones proved in Ref. [13] that the continuum Evans technique gives the same prediction for the bifurcation as Eq. (3). Hence the two methods are consistent, as they should be since they essentially constitute two alternative approaches to a Melnikov calculation [20,21]. Hence, *both* Refs. [19] and [13] concluded the subject at the level of the bifurcation being a power law. No mention of exponentially small terms and their effect appeared in either of these works.

However, in both papers one important aspect of the problem was missed: that there exist two distinct kink solutions to Eq. (1), and the continuum approximation (2) to discreteness does not note this. If one constructs the *exact* discrete static solitons, there are two steady states. When considering the SG equation, the stable steady state corresponds to a (low-energy) kink centered between two consecutive lattice sites, whereas the unstable state corresponds to a (high-energy) kink centered on a lattice site. The exponentially small energy barrier between the two is the celebrated Peierls-Nabarro barrier mirroring the exponential splitting of the heteroclinic orbits. If one performs a numerical linear stability analysis, one finds that for the stable kink a mode bifurcates from the band edge, whereas for the unstable kink no mode appears to bifurcate from the band edge [see, for instance, Fig. 5(b) of Ref. [8], and the relevant explanation]. If the behavior was only a power law and could be described solely by a quartic perturbation, then it should be true that the bifurcation should occur *both* for the stable and unstable modes, since such a continuum-like TI perturbation has no means of discriminating between these two modes. Hence the fact that the behavior of the modes depends on the wave under consideration signifies that there must be terms in a perturbation expansion at a level which discriminates between the two solutions, and consequently it must be an exponentially small effect.

Here we wish to establish that the perturbation expansion for the edge modes detaching from the essential spectrum have exponentially small terms which (a) distinguish between the two different solutions, and (b) can become relevant for sufficiently coarse systems ($d=O(1)$). As a case example, we consider the discrete nonlinear Schrödinger (DNLS) equation

$$iu_{n,t}=-d^2(u_{n+1}+u_{n-1}-2u_n)-2|u_n|^2u_n, \tag{4}$$

which is a rather general model of interest in many of the inherently discrete applications mentioned above. Another reason for this choice is that DNLS equation is a generic envelope equation for Hamiltonian nonlinear lattice systems. Unlike Ref. [14], in which we found the relevant exponentially small term by using the asymptotics beyond all orders (ABAO) technique in the spirit of Hakim and Mallick [22], here we will find this term by using the Evans function. This more general methodology will have the advantage that it will simultaneously pick out the leading order algebraic and exponentially small term for d sufficiently large. An important difference between this work and Ref. [14] is that, for the translational modes, the presence of the continuous symmetry necessitated that to all orders in expansion (2), the frequency of the modes does not bifurcate away from 0 and it is only BAO that the bifurcation occurs. However, the modes studied herein are not associated with some symmetry and, thus, generically the bifurcation will be due to both algebraic and exponential factors, as mentioned above.

In order to perform the perturbation calculation, one must have a well-understood system for large d. In previous works [13,19] the system considered was the continuum NLS equation

$$iu_t+u_{xx}+2|u|^2u+\frac{1}{12d^2}u_{xxxx}=0.$$

The prediction presented therein was that for large d the bifurcating edge mode satisfies the relationship

$$\lambda=i\left(1-\frac{1}{81d^4}\right).$$

As previously remarked, however, this prediction does not distinguish between the two different solutions to the DNLS equation; hence it must be missing some possibly important correction terms.

Instead of using the continuum NLS equation as the approximating system to the DNLS equation, we will use the Ablowitz-Ladik [23,24] discretization of the NLS (AL-DNLS) equation, which is given by

$$iu_{n,t}=-d^2(u_{n+1}+u_{n-1}-2u_n)-|u_n|^2(u_{n-1}+u_{n+1}). \tag{5}$$

The advantage here is that since the AL-DNLS equation is also a discrete system, a perturbation calculation which uses it should naturally pick up all discreteness effects. The AL-DNLS equation is completely integrable; as one consequence, it has an exact solution which is given by

$$U_n(\xi)=\sinh(\alpha)\operatorname{sech}(\tilde{\alpha}n+\xi),$$

where

$$\cosh(\tilde{\alpha})=1+\frac{1}{2d^2},\quad \sinh(\alpha)=d\sinh(\tilde{\alpha}).$$

Note that for d large, $\tilde{\alpha}\approx 1/d$ and $\sinh(\alpha)\approx 1$. It was noted by Herbst and Ablowitz [11] that for d sufficiently large the DNLS equation can be thought of as a perturbation of the AL-DNLS equation. Using this observation, they were able to perform a Melnikov calculation to measure the splitting of the homoclinic orbit. This calculation confirmed the well-known result that for the DNLS equation there exist two solitonlike solutions, both of which are a perturbation of U_n [25]. One solution is a perturbation of $U_n(0)$, and the other is a perturbation of $U_n(\Delta x/2)$. Using the Melnikov calculation of Ref. [11], it can be shown via the construction of the Evans function [26] (as an alternative to the ABAO method of Ref. [14]) that when $\xi=0$ there are no positive eigenvalues of the linear operator near $\lambda=0$, while if $\xi=\Delta x/2$ there is exactly one exponentially small unstable eigenvalue.

The Evans function $E(\lambda)$ is an analytic function of the eigenvalue parameter λ, whose zeros correspond to eigenvalues of the linearized operator [27]. It was recently shown that for continuum problems it is the tool of choice for locating edge modes [28–30]. Furthermore, it is now known that the Evans function is also a useful tool to find eigenvalues for discrete problems [8,26].

For the DNLS equation, the essential spectrum corresponds to a branch cut for the Evans function, with the branch points being at the edges, i.e., at $\lambda=\pm i$ and $\lambda=\pm i(1+4d^2)$. In the problem at hand one would like to write a Taylor expansion for the Evans function near the branch point, and then find the zeros of the resulting series. As already mentioned, these zeros would then be the eigenvalues of the linearized problem. For the rest of this discussion we will focus only on the situation near $\lambda=i$.

In order to perform a Taylor expansion around a branch point, one must define the Evans function on an appropriate Riemann surface. For the DNLS equation, this surface near $\lambda=i$ is defined by

$$\gamma^2=\frac{1+i\lambda}{d^2}\left(1+\frac{1}{4d^2}\right) \tag{6}$$

[26], and is found in the following way. After linearizing Eq. (5) about the wave, one has an eigenvalue problem which can be written as the first-order system

$$\mathbf{Y}_{n+1}=A(\lambda,n)\mathbf{Y}_n,$$

where $\mathbf{Y}_n\in\mathbb{C}^4$. Since the underlying wave decays exponentially fast as $|n|\rightarrow\infty$, one has

$$\lim_{|n|\rightarrow\infty} A(\lambda,n)=A_0(\lambda).$$

Denote the eigenvalues of $A_0(\lambda)$ by $\mu_j^{\pm}(\lambda)$ for $j=1$ and 2, where for $\mathrm{Re}\,\lambda>0$ one has that $\mathrm{Re}\,\mu_j^-(\lambda)<0$ and $\mathrm{Re}\,\mu_j^+(\lambda)>0$. A branch point of the Evans function is determined by the conditions that $\mu_j^-(\lambda)=\mu_j^+(\lambda)$ for some j, and that this eigenvalue for $A_0(\lambda)$ has a geometric multiplicity 1 and an algebraic multiplicity 2. In practice it turns out that the eigenvalue $\mu_j^{\pm}(\lambda)$ also has a branch point when the Evans function does, and the Riemann surface on which the eigenvalues are analytic is also that on which the Evans function is analytic. Once the zeros of the Evans function have been located on the Riemann surface, we take those zeros which lie on the correct sheet, i.e., $\mathrm{Re}\,\gamma>0$, and invert Eq. (6) via

$$\lambda=id^2\left(2+\frac{1}{d^2}-2\sqrt{1+\gamma^2}\right) \tag{7}$$

to find the eigenvalues for the system.

Since the AL-DNLS equation is completely integrable, one can explicitly compute the Evans function associated with it. For example, this was done in Ref. [28] for the focusing NLS equation. In particular, one finds that on the Riemann surface near $\gamma=0(\lambda=i)$ the Evans function satisfies

$$E(0)=0,\quad \partial_\gamma E(0)=4d \tag{8}$$

[26]. Furthermore, one finds that upon using the perturbation techniques established in Refs. [31,28,29] that, with $\epsilon=1/d^2$,

$$\partial_\epsilon E(0)=-\sum_{n=-\infty}^{+\infty} P_n L_\epsilon P_n.$$

In the above equation P_n is the squared eigenfunction at $\lambda=i$ for the linearized operator associated with the AL-DNLS equation, and L_ϵ represents the $O(\epsilon)$ correction of that operator when perturbing to the DNLS equation. An evaluation of the above sum yields

$$\partial_\epsilon E(0)=-\left[\frac{4}{9}+C(d)e^{-\pi^2/\tilde{\alpha}}\cos\left(\frac{2\pi\xi}{\tilde{\alpha}}\right)\right], \tag{9}$$

where, to lowest order,

$$C(d)=\frac{256\pi}{45}\left(\frac{\pi}{\tilde{\alpha}}\right)^7\approx 53979.2d^7.$$

In Eq. (9), ξ can take the values 0 (corresponding to the stable wave) and $1/(2d)$ (corresponding to the unstable wave). It is important to note here that (a) the exponentially small term distinguishes between the two solutions, and (b) although the exponentially small term is numerically negligible for d sufficiently large, it begins to have an $O(1)$ effect for $d\leqslant 2.0$.

As a consequence of Eqs. (8) and (9), the Evans function has an expansion on the Riemann surface which is given by

$$E(\gamma,d)=4d\left[\gamma-\frac{1}{9d^3}\left\{1+\frac{9}{4}C(d)e^{-\pi^2/\tilde{\alpha}}\cos\left(\frac{2\pi\xi}{\tilde{\alpha}}\right)\right\}\right]. \tag{10}$$

For d sufficiently large the zero of the Evans function on the Riemann surface is positive; hence, by using the inversion relationship (7) one obtains that the eigenvalue satisfies

$$\lambda(\xi)=i\left[1-\frac{1}{81d^4}\left\{1+\frac{9}{2}C(d)e^{-\pi^2/\tilde{\alpha}}\cos\left(\frac{2\pi\xi}{\tilde{\alpha}}\right)\right\}\right]. \tag{11}$$

It is now seen that for d sufficiently large the locations of the edge modes associated with $\xi=0$ and $\xi=1/(2d)$ differ by an

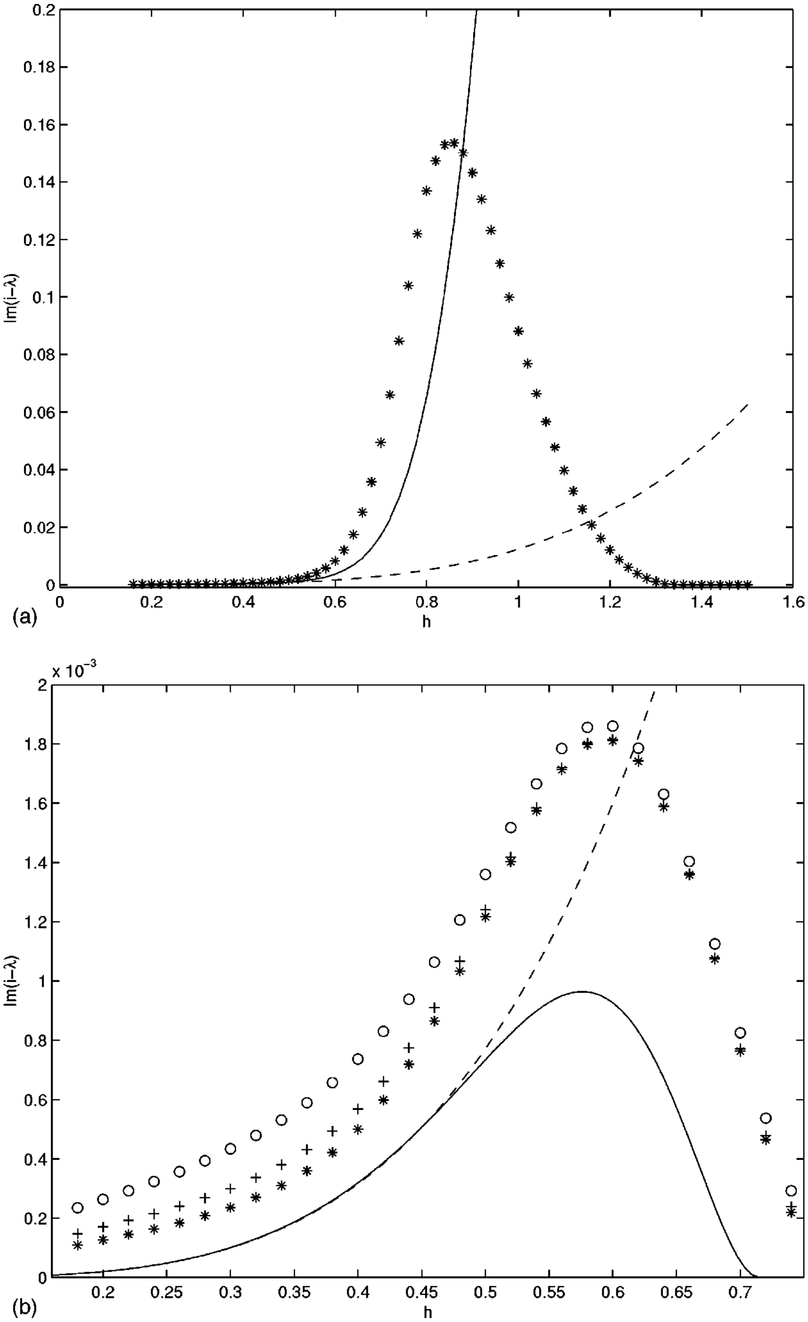

FIG. 1. For the top and bottom panel (for the stable and unstable wave, respectively), the dashed line shows the theory of Ref. [19], the solid line the theory of this paper, and the stars the results of numerical experiments on a 400-site lattice with PBC's. In the bottom panel, circles indicate results on a 200-site lattice and pluses results on a 300-site lattice.

exponentially small amount, and that the edge mode associated with $\xi=0$ drops faster than that associated with $\xi=1/(2d)$.

Hence one has a clear explanation for the disparity between theory and numerical experiment in Fig. 1 of Ref. [19], as well as for the discrimination between the two steady states with respect to their breathing eigenmodes. Each algebraic term in the perturbation expansion for the edge mode, i.e., $\partial_\epsilon^k E(0)$ for $k \geqslant 2$, possesses an exponentially small correction which distinguishes between the two solutions; furthermore, each of these small correction terms becomes significant for $d=O(1)$. Hence, for $d=O(1)$ the coefficients in the two expansions are no longer close to each other, which implies that one can get the observed behavior.

This analysis is illustrated in the two panels of Fig. 1. The top panel shows the bifurcation for the stable wave as predicted by the two theories (the single power law of Ref. [19], given by dashed line, as well as the power law with exponential corrections, shown by the solid line) compared with the numerical experiment (stars). The significantly better agreement of the theory that includes the exponential corrections is clearly illustrated. Even more dramatic in the contrast of the predictions of the two theories is the lower panel, indicating the bifurcation of the unstable wave. Here the difference in scale in the two bifurcations (of the top and bottom panel for the stable and unstable wave) should be highlighted (the maximal bifurcation for the stable wave is ≈ 0.155, whereas for the unstable it is ≈ 0.0019). It should be noted that the theory of Ref. [19] *cannot* distinguish between bifurcation for the two waves, and is clearly unable to capture such effects (as is any power law TI type of scheme). Additionally, the exponentially small correction captures the effect of the mode returning to the band edge at finite $h = 1/d$ (due to the competition between the power law and the exponential factors), another phenomenon which is not visible to pure power law perturbations. Note that this is the first time, to our knowledge, that the contribution of exponentially small terms in this bifurcation has been appreciated (especially for coarse lattices that are used for the applications involving discrete systems). Furthermore, we believe it is the first time that these effects have been quantified to leading exponential order, giving good agreement even for strongly discrete systems. This is contrary to the consistent but insufficient power law theoretical descriptions of Refs. [19] and [13]. The discrepancies between the numerical experiment and our theory are expected to be due to the higher order contributions as well as partly (especially in the unstable wave case) due to finite size effects. The finite size of the lattice, as also observed in Ref. [8], causes corrections (close to the continuum limit) of $O(10^{-4})$ in the eigenvalues. This is (almost) negligible for the stable wave, but for the unstable wave it is clearly observable and is shown in the lower panel of Fig. 1, where the circles indicate numerical calculations with periodic boundary conditions (PBC's) on a 200-site lattice, the pluses the same on a 300-site lattice, and the stars the same on a 400-site lattice. These additional factors being considered, we can conclude that even though power law effects are important when studying bifurcations close to the band edge (contrary to what is true close to the origin [14]), it is crucial to properly incorporate exponentially small corrections to obtain a good agreement with and an understanding of the numerical observations.

It should be noted that similar results can be found for the sine Gordon equation and the ϕ^4 equation (for their corresponding integrable discretizations). Alternatively, exponentially small phenomena such as the ones discussed here can be captured by the ABAO method [22,32,33,14]. The results are similar to the ones given here, and will be presented elsewhere.

For very strong discreteness, i.e., for $h \gg 1$, neither the ABAO nor Evans methods can capture the actual behavior of the (stable) mode very well. While this is to be expected, extending the theoretical methodology to the regime of very strong discreteness ($d \ll 1$) remains an outstanding mathematical challenge that will be left for future studies.

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