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Length scale competition in nonlinear Klein—Gordon models: A collective coordinate approach

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Working within the framework of nonlinear Klein–Gordon models as a paradigmatic example, we show that length scale competition, an instability of solitons subjected to perturbations of an specific length, can be understood by means of a collective coordinate approach in terms of soliton position and width. As a consequence, we provide a natural explanation of the phenomenon in much simpler terms than any previous treatment of the problem. Our technique allows us to study the existence of length scale competition in most soliton bearing nonlinear models and can be extended to coherent structures with more degrees of freedom.
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Solitons, solitary waves, vortices, and other coherent structures possess, generally speaking, a characteristic length or size. One important feature of these coherent structures, which usually are exact solutions of certain nonlinear models, is their robustness when the corresponding models are perturbed in different ways. A case relevant in many real applications is that of space-dependent perturbations, which may or may not have their own typical length scale. Interestingly, in the latter case, it has been known for a decade that when the perturbation length scale is comparable to the size of the coherent structures, the effects of even very small perturbing terms are dramatically enhanced. Although some analytical approaches have shed some light on the mechanisms for this special instability, a clear-cut, simple explanation was lacking. In this paper, we show how such explanation arises by means of a reduction of degrees of freedom through the so-called collective coordinate technique. The analytical results have a straightforward physical interpretation in terms of a resonant-like phenomenon. Notwithstanding the fact that we work on a specific class of soliton-bearing equations, our approach is readily generalizable to other equations and/or types of coherent structures.

I. INTRODUCTION

Fifty years after the pioneering discoveries of Fermi, Pasta, and Ulam,[1] the paradigm of coherent structures has proven itself one of the most fruitful ones of nonlinear science.[2] Fronts, solitons, solitary waves, breathers, and vortices are instances of such coherent structures of relevance in a plethora of applications in very different fields. One of the chief reasons that gives all these nonlinear excitations their paradigmatic character is their robustness and stability: Generally speaking, when systems supporting these structures are perturbed, the structures continue to exist, albeit with modifications in their parameters or small changes in shape (see Refs. 3 and 4 for reviews). This property that all these objects (approximately) retain their identity allows one to rely on them to interpret the effects of perturbations on general solutions of the corresponding models.

Among the different types of coherent structures one can encounter, topological solitons are particularly robust due to the existence of a conserved quantity named topological charge. Objects in this class are, e.g., kinks or vortices and can be found in systems ranging from Josephson superconducting devices to fluid dynamics. A particularly important representative of models supporting topological solitons is the family of nonlinear Klein–Gordon equations,[2] whose expression is

$$\phi_{tt} - \phi_{xx} + \frac{dU}{d\phi} = 0. \tag{1}$$

Specially important cases of this equation occur when $U(\phi)=\frac{1}{4}(\phi^2-1)^2$, giving the so-called ϕ^4 equation, and when $U(\phi)=1-\cos(\phi)$, leading to the sine-Gordon (sG) equation, which is one of the few examples of fully integrable systems.[5] Indeed, for any initial data the solution of the sine-Gordon equation can be expressed as a sum of kinks (and antikinks), breathers, and linear waves. Here we focus on kink solitons, which have the form

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$$\phi(x,t) = 4\arctan\left\{\exp\left(\frac{x-vt}{\sqrt{1-v^2}}\right)\right\}, \tag{2}$$

$0 \leqslant v < 1$ being a free parameter that specifies the kink velocity. The topological character of these solutions arises from the fact that they join two minima of the potential $U(\phi)$, and therefore they cannot be destroyed in an infinite system. Our other example, the ϕ^4 equation, is not integrable, but supports topological, kinklike solutions as well, given by

$$\phi(x,t) = \tanh\left(\frac{x-vt}{\sqrt{2(1-v^2)}}\right). \tag{3}$$

It is by now well established already from pioneering works in the 1970s[6,7] that both types of kinks behave, under a wide class of perturbations, like relativistic particles. The relativistic character arises from the Lorentz invariance of their dynamics, see Eq. (1), and implies that there is a maximum propagation velocity for kinks (1 in our units) and their characteristic width decreases with velocity. Indeed, even behaving as particles, kinks do have a characteristic width; however, for most perturbations, that is not a relevant parameter and one can consider kinks as pointlike particles. This is not the case when the perturbation itself gives rise to a certain length scale of its own, a situation that leads to the phenomenon of length scale competition, first reported in Ref. 8 (see Ref. 9 for a review). This phenomenon is nothing but an instability that occurs when the length of a coherent structure approximately matches that of the perturbation: Then, small values of the perturbation amplitude are enough to cause large modifications or even destroy the structure. Thus, in Ref. 8, the perturbation considered was sinusoidal, of the form

$$\phi_{tt} - \phi_{xx} + \frac{dU}{d\phi}(1+\epsilon\cos(kx)) = 0, \tag{4}$$

where ϵ and k are arbitrary parameters. The structures studied here were breathers, which are exact solutions of the sine-Gordon equation with a time-dependent, oscillatory mode (hence the name "breather") and that can be seen as a bound kink-antikink pair. It was found that small k values, i.e., long perturbation wavelengths, induced breathers to move as particles in the sinusoidal potential, whereas large k or equivalent short perturbation wavelengths λ were unnoticed by the breathers. In the intermediate regime, where length scales were comparable, breathers (which are nontopological) were destroyed.

As breathers are quite complicated objects, the issue of length scale competition was addressed for kinks in Ref. 10. In this case, kinks were not destroyed because of the conservation of the topological charge, but length scale competition was present in a different way: Keeping all other parameters of the equation constant, it was observed that kinks could not propagate when the perturbation wavelength was of the order of their width. In all other (smaller or larger) perturbations, propagation was possible and, once again, easily understood in terms of an effective pointlike particle. Although an explanation of this phenomenon was provided in Ref. 10 in terms of a (numerical) linear stability analysis and the radiation emitted by the kink, it was not a fully satisfactory argument for two reasons: First, the role of the kink width was not at all transparent, and, second, there were no simple analytical results. These are important issues because length scale competition is a rather general phenomenon: It has been observed in different models (such as the nonlinear Schrödinger equation[11]) or with other perturbations, including random ones.[12] Therefore, having a simple, clear explanation of length scale competition will be immediately of use in those other contexts.

The aim of the present paper is to show that length scale competition can be understood through a collective coordinate approximation. Collective coordinate approaches were introduced in Refs. 6 and 7 to describe kinks as particles (see Refs. 2–4 and 9 for a very large number of different techniques and applications of this idea). Although the original approximation was to reduce the equation of motion for the kink to an ordinary differential equation for a time-dependent, collective coordinate which was identified with its center, it is being realized lately that other collective coordinates can be used instead of or in addition to the kink center. One of the most natural additional coordinates to consider is the kink width, an approach that has already produced new and unexpected results such as the existence of anomalous resonances[13] or the rectification of ac drivings.[14] There are also cases in which one has to consider three or more collective coordinates (see, e.g., Ref. 15). It is only natural then to apply these extended collective coordinate approximations to the problem of length scale competition, in search for the analytical explanation needed. As we will see below, taking into account the kink width dependence on time is indeed enough to reproduce the phenomenology observed in the numerical simulations. Our approach is detailed in Secs. II and III, whereas in Sec. IV we collect our results and discuss our conclusions.

II. COLLECTIVE COORDINATE APPROACH

We now present our collective coordinate approach to the problem of length scale competition for kinks.[10] We will use the Lagrangian-based approach developed in Ref. 16, which is very simple and direct. Equivalent results can be obtained with the so-called generalized traveling wave *ansatz*,[17] somewhat more involved in terms of computation but valid even for systems that cannot be described in terms of a Lagrangian.

Let us consider the generically perturbed Klein–Gordon equation:

$$\phi_{tt} - \phi_{xx} + \frac{dU}{d\phi} + \epsilon f(x,t)g(\phi) = 0. \tag{5}$$

The starting point of our approach is the Lagrangian for the above equation, which is given by

$$L = \int_{-\infty}^{\infty} dx \left\{ \frac{1}{2}\dot{\phi}^2 - \frac{1}{2}\phi_x^2 - U(\phi) + \epsilon g(\phi)\phi_x \int_{x_0}^{x} dy f(y,t) \right\}. \tag{6}$$

We stress that the approach we are presenting here is fairly general and, notwithstanding the fact that we have specific choices for the functions f and g in mind, the Lagrangian (6) can be used to study any other problem given by different functions, by following exactly the same formalism we present below.

As stated above, we now focus on the behavior of kink excitations of the form (3) and (2). To do so, we will use a two collective coordinate approach by substituting the *ansatz*

$$\phi(z(t)) = \tanh(z(t)) \tag{7}$$

in the Lagrangian of the ϕ^4 system and

$$\phi(z(t)) = 4\arctan\{\exp(z(t))\} \tag{8}$$

in *sG*, where $z(t)=[x-X(t)]/l(t)$ and $X(t)$ and $l(t)$ are two collective coordinates that represent the position of the center and the width of the kink, respectively. Substituting the expressions (7) and (8) in the Lagrangian (6) with our perturbation, $f(x,t)=\cos(kx)$ and $g(\phi)=dU/d\phi$, we obtain an expression of the Lagrangian in terms of X and l,

$$L = \frac{M_0 l_0}{2l}\dot{X}^2 + \frac{\alpha M_0 l_0}{2l}\dot{l}^2 - \frac{M_0}{2}\left(\frac{l_0}{l} + \frac{l}{l_0}\right) - \frac{\epsilon}{k}\cos(kX)w(kl), \tag{9}$$

where, for the ϕ^4 system, $M_0=4/(3\sqrt{2})$, $l_0=\sqrt{2}$, and $\alpha=(\pi^2-6)/12$, and for the sG system, $M_0=8$, $l_0=1$, and $\alpha=\pi^2/12$, and

$$w(x) = \int_{-\infty}^{\infty} dz \tanh(z)(\phi'(z))^2 \sin(xz), \tag{10}$$

which is

$$w(x) = \frac{\pi x^2(x^2+4)}{24\sinh(\pi x/2)} \tag{11}$$

for ϕ^4 and

$$w(x) = \frac{2\pi x^2}{\sinh(\pi x/2)} \tag{12}$$

for the sG model. We note that the effect of a spatially periodic perturbation like the one considered here was studied for the ϕ^4 model in Ref. 18, although the authors were not aware of the existence of length scale competition in this system and focused on unrelated issues.

The equations of motion of X and l can now be obtained using the Lagrange equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{Y}_i}\right) = \frac{\partial L}{\partial Y_i}, \tag{13}$$

where Y_i stands for the collective coordinates X and l. The ordinary differential equation (ODE) system for X and l is, finally,

$$\dot{P} = \epsilon \sin(kX)w(kl), \tag{14}$$

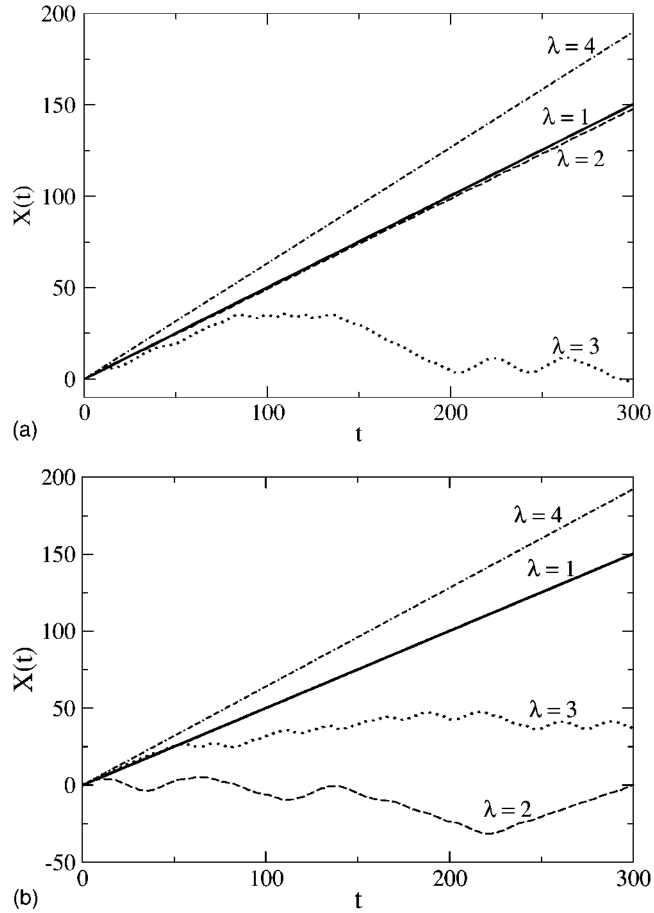

FIG. 1. Different behaviors of $X(t)$ for different values of $\lambda=2\pi/k$ for $\epsilon=0.7$, $X(0)=0$, $\dot{X}(0)=0.5$, $l(0)=l_0(1-\dot{X}(0)^2)^{1/2}$, and $\dot{l}(0)=0$ in the (a) sG model and (b) ϕ^4 model.

$$\dot{Q} = -\frac{1}{2M_0 l_0}\left(P^2 + \frac{Q^2}{\alpha}\right) + \frac{M_0 l_0}{2}\left(\frac{1}{l^2} - \frac{1}{l_0^2}\right) - \epsilon\cos(kX)w'(kl), \tag{15}$$

where $P=M_0 l_0 \dot{X}/l$ and $Q=\alpha M_0 l_0 \dot{l}/l$.

III. COMPARISON WITH NUMERICAL SIMULATIONS

The equations above are our final result for the dynamics of sG and ϕ^4 kinks in terms of their center and width. As can be seen, they are quite complicated equations and we have not been able to solve them analytically. Therefore, in order to check whether or not they predict the appearance of length scale competition, we have integrated them numerically using a Runge-Kutta scheme.[19] The simulation results for different values of $\lambda=2\pi/k$ are in Fig. 1. Motivated by the results presented in Ref. 10, we begin by considering a large perturbation value, namely $\epsilon=0.7$. The plots present already the physical variable $X(t)$, i.e., the position of the center of the kink. The validity of the collective coordinate results is assessed in Fig. 2, which presents numerical simulations, using a fourth-order Runge-Kutta scheme, of both the full sG and ϕ^4 partial differential equations. For small and large wavelengths the kink, initially at the top of one of the maxima of the perturbation, travels freely; however, for in-

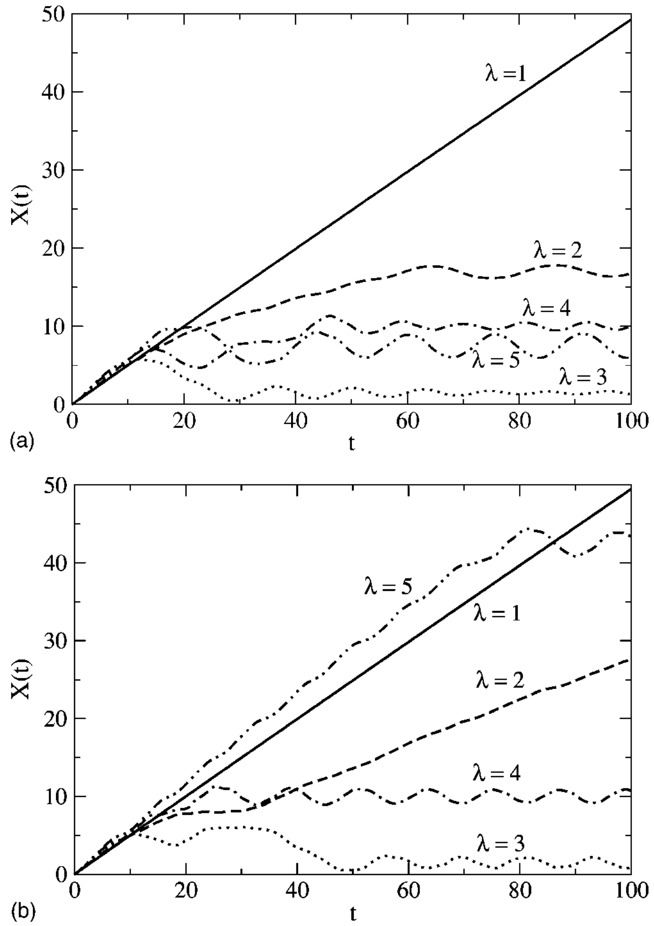

FIG. 2. Different behaviors of $X(t)$ for different values of $\lambda=2\pi/k$ for $\epsilon=0.7$, $X(0)=0$, and $\dot{X}(0)=0.5$ as obtained from numerical simulations of the full (a) sG and (b) ϕ^4 models.

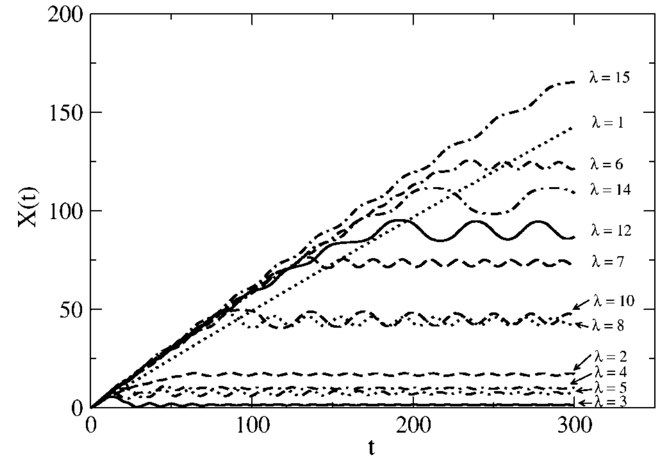

FIG. 3. Same as Fig. 2(a), but for longer times and more perturbation wavelengths. Only results of numerical simulations for the sG equation are presented.

termediate scales, the kink is trapped and even moves backward for a while. We note in passing that this agrees with the results for the sG equation in Ref. 10 (cf. Figs. 7 and 8 in Ref. 10).

Analyzing the simulation results in more detail, we see that for both equations and for λ values around 2 or 3, the kink is trapped at the first few potential wells (the first one for $\lambda=3$), indicating that for that value the length scale competition phenomenon is close to its maximum effect. It is clear from Fig. 1 that the prediction of the collective coordinate approach is qualitatively correct, but the full equations show the length scale competition phenomena in a wider range of wavelengths. We will come back to this question below, but at this time we want to highlight the physical mechanism behind the instability. There is not any single criterion to define the "length" or "width" of the kink solutions of nonlinear Klein–Gordon equations: One can take, for instance, the point at which the midheight of the kink has decreased by a factor *e*, or the width at half maximum of the kink derivative with respect to *x*. While those numbers do not exactly agree, they yield values for the kink width around 2.5, i.e., the same value at which collective coordinates predict the appearance of length scale competition and at which the numerical simulations show the most dramatic effects. Therefore, we can naturally understand this instability as a resonancelike phenomenon between the width of the kink and the length scale of the perturbation (and hence the name length scale competition).

Interestingly, if we look at longer times and a wider range of wavelengths, as depicted in Fig. 3 for the sG equation, we can distinguish two different kink trapping processes. In agreement with the collective coordinate prediction, for the range of $\lambda=2,3$ discussed above, we observe that the kink is trapped very early, after having traveled a few potential wells at most [note that the trajectories plotted in Fig. 2(a) are all grouped at the bottom of Fig. 3]. This is the length scale competition regime. However, there is an additional trapping mechanism: As is well known,[18] kinks traveling on a periodic potential emit radiation. This process leads to a gradual slowing down of the kink until it is finally unable to proceed over a further potential well. This takes place at a much slower rate than length scale competition and hence the kink is stopped after traveling a larger distance in the system. The radiation emission as observed in the simulation is smoother than in the length scale competition trapping. In fact, radiation is present at any value of the perturbative wavelength, this being the reason why the collective coordinate prediction for the range in which length scale competition is observed is smaller than in the numerical simulations: Indeed, by construction, the analytical approach cannot account for the energy that the kink disspates in the form of radiation. In the full partial differential equation, however, kinks propagating in perturbations of lengths close to the resonant one (such as $\lambda=4,5$) radiate a fair amount of energy, becoming trapped after a few potential wells.

The above paragraph brings out the need for a closing discussion of the accuracy of our perturbative approach. We have focused on large values of the perturbation because of our previous work on this subject,[10] and we have found a qualitative agreement between the collective coordinate approach and the full numerical simulations. Is the agreement qualitative for smaller perturbations? Before answering this question, let us clarify that the collective coordinate technique is more a variational than a standard perturbative pro-

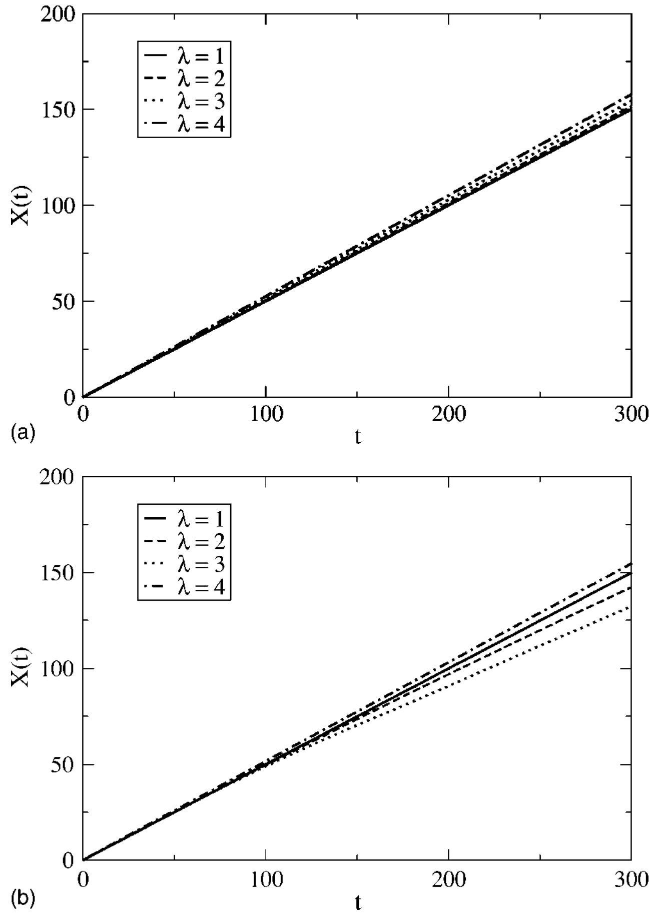

FIG. 4. Different behaviors of $X(t)$ for different values of $\lambda=2\pi/k$ for $\epsilon=0.1$, $X(0)=0$, and $\dot{X}(0)=0.5$ as predicted by the collective coordinate approach (left) and as obtained from numerical simulations (right) of the sG model.

cedure, and there is not any small parameter that can be used to control the approximation. However, it is of course to be expected that the smaller the perturbation, the better the predictions. Figure 4 shows that this is indeed the case, for the same value of the initial velocity as above but for a perturbation $\epsilon=0.1$. We see that in this case the agreement is quantitatively correct to a few percent, while showing the fact, already observed in Ref. 10, that for these velocities there is no length scale competition when the perturbing potential is small [we have found length scale competition and a very similar scenario to the one discussed above for $\epsilon=0.1$ when $\dot{X}(0)=0.005$ (not shown)]. It is interesting to note, however, that the agreement is worse for $\lambda=2,3$, which signals the fact that, even if it is not observed for this set of parameters, the length scale competition instability is influencing the system behavior. In any event, the accuracy of the collective coordinate approach does improve for smaller perturbations in general, although we believe that its main achievement in this case is the prediction of the appearance or not of length scale competition.

IV. DISCUSSION AND CONCLUSIONS

As we have seen in the preceding section, a collective coordinate approach in terms of the kink center and width is able to explain the phenomenon of length scale competition, observed in numerical simulations earlier for the sG equation with a spatially periodic perturbation.[9,10] The structure of the equations makes clear the necessity for a second collective coordinate; imposing $l(t)=l_0$ constant, we recover the equation for the center already derived in Ref. 10, which shows no sign at all of length scale competition, predicting effective particlelike behavior for all λ. The validity of this approach has been also shown in the context of the ϕ^4 equation, which had not been considered before from this viewpoint. In spite of the fact that the collective coordinate equations cannot be solved analytically, they provide us with the physical explanation of the phenomenon in so far as they reveal the key role played by the width changes with time and their coupling with the translational degree of freedom. They have also allowed us to confirm that length scale competition is not present in situations where the perturbation is smaller while keeping the same initial velocity. This shows that our approach does capture a great deal of the physical mechanisms involved in this instability. Finally, we have also analyzed the accuracy of the collective coordinate technique in quantitative terms, tracing the discrepancies to the effect of radiation, which is not included in our approximation.

It is interesting to reconsider the analysis carried out in Ref. 10 of length scale competition through a numerical linear stability analysis. In that previous work, it was argued that the instability arose because, for the relevant perturbation wavelengths, radiation modes moved below the lowest phonon band, inducing the emission of long wavelength radiation which in turn led to the trapping of the kink. It was also argued that those modes became internal modes, i.e., kink shape deformation modes in the process. The approach presented here is a much more simple way to account for these phonon effects: Indeed, as was shown by Quintero and Kevrekidis,[20] (odd) phonons do give rise to width oscillations very similar to those induced by an internal mode.[20] We are confident that what our perturbation technique is making clear is precisely the result of the action of those phonons, summarized in our approach in the width variable $l(t)$. The case for the ϕ^4 equation is slightly different: Whereas the sG kink does not have an internal mode[21] and $l(t)$ is hence a collective description of phonon modes, the ϕ^4 kink possesses an intrinsic internal mode that is easily excited by different mechanisms (such as interaction with inhomogeneities[22–26]). Therefore, one would expect that for the ϕ^4 equation the effect of a perturbation of a given length is more dramatic than for the sG model, as indeed is the case: See Fig. 1 for a comparison, showing that the kink is trapped for a wider range of values of λ in the ϕ^4 equation. Remarkably, the present and previous results using this two collective coordinate approach, and particularly their interpretation in terms of phonons, suggest that this technique could be something like a "second-order collective coordinate perturbation theory," the width degree of freedom playing the role of the second-order term. We believe it is appealing to explore this possibility from a more formal viewpoint; if this idea is correct, then one could think of a scheme for adding in a standard way as many collective coordinates as needed to achieve the required accuracy. Progress in that direction would provide the necessary mathematical grounds for this fruitful approximate technique.

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