

Four Decades of Kink Interactions in Nonlinear Klein-Gordon Models: A Crucial Typo, Recent Developments and the Challenges Ahead

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The study of kink interactions in nonlinear Klein-Gordon models in 1 + 1-dimensions has a time-honored history. Until a few years ago, it was arguably considered a fairly mature field whose main phenomenology was well understood both qualitatively and at least semi-quantitatively. This consensus was shattered when H. Weigel and his group established that the effective model that had allowed this detailed understanding contained an all-important typo. Remarkably, they found that correcting this error wipes out both the quantitative and qualitative agreement and, in fact, leads to additional problems. We summarize the history of the subject from the early studies, up to Weigel's work and reflect on where these recent developments leave our understanding (which, quantitatively, is close to square one!). Importantly, we stress a number of emerging additional directions that have arisen in higher-order power law models and speculate on the associated significant potential for future work.

I. PREAMBLE TEASER: A MISTAKE!

Intriguingly, mathematics and science occasionally benefit significantly from a mistake that propels an area forward. Arguably, the most famous such example is the mistake in Poincaré's entry in the competition to construct a convergent series solution to the three-body gravitational problem, sponsored by King Oscar II of Sweden and Norway. After accepting the prize, Poincaré discovered a significant problem with his calculations. This, in turn, led him to discover the phenomena of sensitive dependence on initial conditions and chaos. Diacu and Holmes beautifully chronicle this story in [20] and we recommend it to anyone working in Dynamical Systems, as it describes, effectively, the genesis of the field.

Our exposition is centered around another mistake of this kind. It, in fact, appears far more innocuous-looking, as it only concerns an apparent typographical error. Yet, it has proved so detrimental that it has set a seemingly mature and well-understood field in complete disarray: much of the qualitative and semi-quantitative theory can, remarkably, no longer be considered applicable (except in a phenomenological way). But let us go back to the beginning.

II. IN THE BEGINNING, THERE WAS INTEGRABILITY...

In the 1970's, the discovery of the magical-seeming theory of completely integrable nonlinear waves revolutionized the study of nonlinear waves and led to a Steele Prize for its founders [1]. The centerpiece of this theory, the inverse scattering transform (IST), has since been summarized in numerous books [2, 5, 23]. A major consequence of this theory is that the interaction of solitary waves is *perfectly elastic* in integrable field theories, most notably in the many 1+1 dimensional examples. Solitary waves in such systems are called solitons and emerge from collisions with their form and velocity unchanged, modulo a so-called phase shift (a displacement from their undisturbed trajectory). Relevant examples include nonlinear Klein-Gordon equations such as the famous sine-Gordon (sG) equation [18, 21]

$$u_{tt} = u_{xx} - \sin(u), \tag{1}$$

which arises in models of superconducting Josephson junctions, coupled torsion pendula, and surfaces of constant negative curvature (among many other applications). Remarkably, similar behavior arises in the universal nonlinear Schrödinger equation [4, 39] used to model fluids and superfluids, optics and plasmas, and many other applications. Note that x and t subscripts will be used hereafter to denote space and time partial derivatives, while u will be used to denote the spatio-temporally dependent field.

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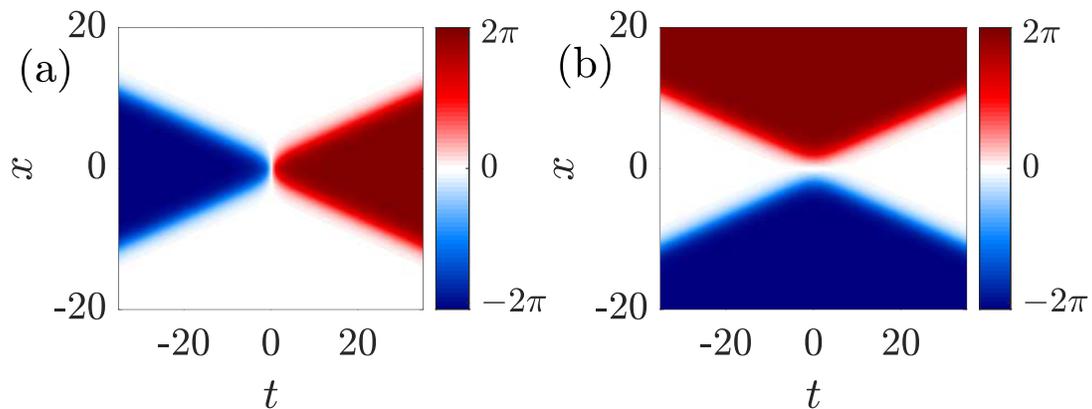


FIG. 1: (a) The kink-antikink solution and (b) the kink-kink solution, both with $v = 0.28$.

Simple dynamical systems methods show that the sG model possesses single-soliton solutions in the form of kinks:

$$u_K(x, t) = 4 \tan^{-1} \left(e^{\frac{x-x_0-vt}{\sqrt{1-v^2}}} \right), \quad -1 < v < 1, \quad (2)$$

and antikinks $u_{\bar{K}}(x, t) = u_K(-x, t)$. These two solutions are simply heteroclinic orbits connecting the spatially homogeneous solutions given by stable fixed points, and are centered initially at x_0 , or $-x_0$ in the above antikink definition, and potentially traveling with speed v as a result of Lorentz invariance. The IST methods leveraged the miracles of complete integrability (such as their surprising nonlinear superposition principles) to construct from simpler single-kink solutions, more elaborate ones such as kink-antikink and kink-kink solutions, in the form:

$$u_{K\bar{K}}(x, t) = 4 \tan^{-1} \left(\frac{\sinh \frac{vt}{\sqrt{1-v^2}}}{v \cosh \frac{x}{\sqrt{1-v^2}}} \right), \quad u_{KK}(x, t) = 4 \tan^{-1} \left(\frac{v \sinh \frac{x}{\sqrt{1-v^2}}}{\cosh \frac{vt}{\sqrt{1-v^2}}} \right). \quad (3)$$

These are plotted in Fig. 1. Although it may not appear obvious from the formulas, at long times these solutions asymptotically separate, respectively, into the sum of a kink and anti-kink and the sum of two kinks.

Such exact solutions allow us to infer that kinks and anti-kinks attract each other dynamically, while two kinks repel, as shown by the following simple but entertaining calculation. As a single kink runs from $u = 0$ to $u = 2\pi$, its center is considered to be located at $u = \pi$. Then, $u_{K\bar{K}} = \pi$ leads to

$$\tan \left(\frac{u}{4} \right) = \frac{\sinh \frac{vt}{\sqrt{1-v^2}}}{v \cosh \frac{x}{\sqrt{1-v^2}}} \Rightarrow v \cosh \left(\frac{x}{\sqrt{1-v^2}} \right) = \sinh \left(\frac{vt}{\sqrt{1-v^2}} \right). \quad (4)$$

Assuming $v \ll 1$ (i.e., the Newtonian, rather than relativistic regime) and working in the sector $x \gg 1$, $t \gg 1$, we may extract the equation for the center located at x :

$$x = -\log(v) + vt - e^{-2vt} \Rightarrow \ddot{x} = -4e^{-2x}, \quad V_{\text{eff}}(s) = -32e^{-s}. \quad (5)$$

To define the kinetic and potential energy of kink-antikink attraction, we have introduced the separation, $s = 2x$, and the notion of kink mass,

$$M = \int u_x^2 dx, \quad (6)$$

which in the sG case equals 8. We can immediately infer the attractive nature of the interaction from the sign of $V'(x)$. An equivalent calculation finds repulsion in the case of kink-kink interaction.

This simple calculation yields important insights, but at the same time, it is quite special and can be performed as such only in the case of integrable models. Unfortunately, most realistic applications do not yield integrable models, and are not amenable to methods based on exact solutions. As a result, we must develop techniques that work beyond the strict confines of integrable settings.

III. THEN A GENERALIZATION: NONINTEGRABLE KLEIN-GORDON MODELS

Nonlinear Klein-Gordon PDEs are the natural generalization of the sG equation, taking the form:

$$u_{tt} = u_{xx} - V'(u). \quad (7)$$

Many important examples have been studied, most famously the sG equation, stemming from the potential $V(u) = 1 - \cos(u)$ and the ϕ^4 model [31], for which $V(u) = \frac{1}{2}(1 - u^2)^2$. The ϕ^4 -system will be at the epicenter of the next few sections, as attempts to understand its dynamics led to the mistake motivating this article. The ϕ^4 model is often considered as a prototypical system for phase transitions, ferroelectrics, high-energy physics and other applications [21, 31].

Importantly, many of these models have exact solutions such as kinks; in the ϕ^4 case, for example, they interpolate between the temporally stable fixed points of $u = +1$ and -1 (or vice versa) and have the explicit functional form:

$$u_K(x, t) = \tanh\left(\frac{x - x_0 - vt}{\sqrt{1 - v^2}}\right), \quad u_{\bar{K}}(x, t) = -u_K(x, t). \quad (8)$$

In [34], Manton constructed a method to characterize the interaction between kinks (and antikinks) that applies to Hamiltonian wave equations, both integrable and non-integrable. We briefly review it here. Models such as Eq. (7) conserve various quantities, i.e. leave them unchanged over time. These include the energy

$$H = \int_{-\infty}^{\infty} \frac{1}{2}u_t^2 + \frac{1}{2}u_x^2 + V(u)dx \quad (9)$$

and the momentum

$$P = - \int_{-\infty}^{\infty} u_t u_x dx. \quad (10)$$

If we consider the momentum contained between two locations $x = a$ and $x = b$, rather than between $-\infty$ and ∞ , we can directly derive, using Eq. (7),

$$\frac{dP}{dt} = \left[-\frac{1}{2}u_t^2 - \frac{1}{2}u_x^2 + V(u) \right]_a^b \quad (11)$$

If we now assume an anti-kink at $x = 0$ and a kink at $x = s$, then we can approximate the waveform of their superposition (more on this approximation later) as:

$$u = u_1(x) + u_2(x) + c, \quad u_1(x) = u_K(-x), \quad u_2(x) = u_K(x - s) \quad (12)$$

where the K subscript has been again used to denote the kink nature of the waveforms. Then, under the assumption that $a \ll 0 \ll b \ll s$,

$$\frac{dP}{dt} \approx \left[-\frac{1}{2}u_{1x}^2 - u_{1x}u_{2x} + V(u_1) + V'(u_1)u_2 \right]_a^b. \quad (13)$$

The contributions to the momentum change due to the interaction between the two waves stem from the 2nd and 4th terms and hence using the kink asymptotics $u_1 \approx -c + A \exp(-mx)$ and $u_2 \approx -c + A \exp(m(x - s))$ (for sG $m = 1$ and $A = 4$), we obtain

$$\frac{dP}{dt} = 2A^2m^2 \exp(-ms) \Rightarrow V_{\text{eff}}(s) = -2A^2m \exp(-ms) \quad (14)$$

leading to the equation of motion $\ddot{s} = -\frac{2}{M} \frac{dP}{dt}$ for the general Klein-Gordon case. In the sG case, this calculation produces the same result found in the previous section, while in the non-integrable ϕ^4 case, it gives $\ddot{x} = -16 \exp(-2x)$. That is to say, well-separated kinks and antikinks still attract each other and would collide accordingly. Moreover, the above methodology of [34] can be generalized broadly to nonlinear wave systems in which the forms of the waves (or at least their asymptotics) are known.

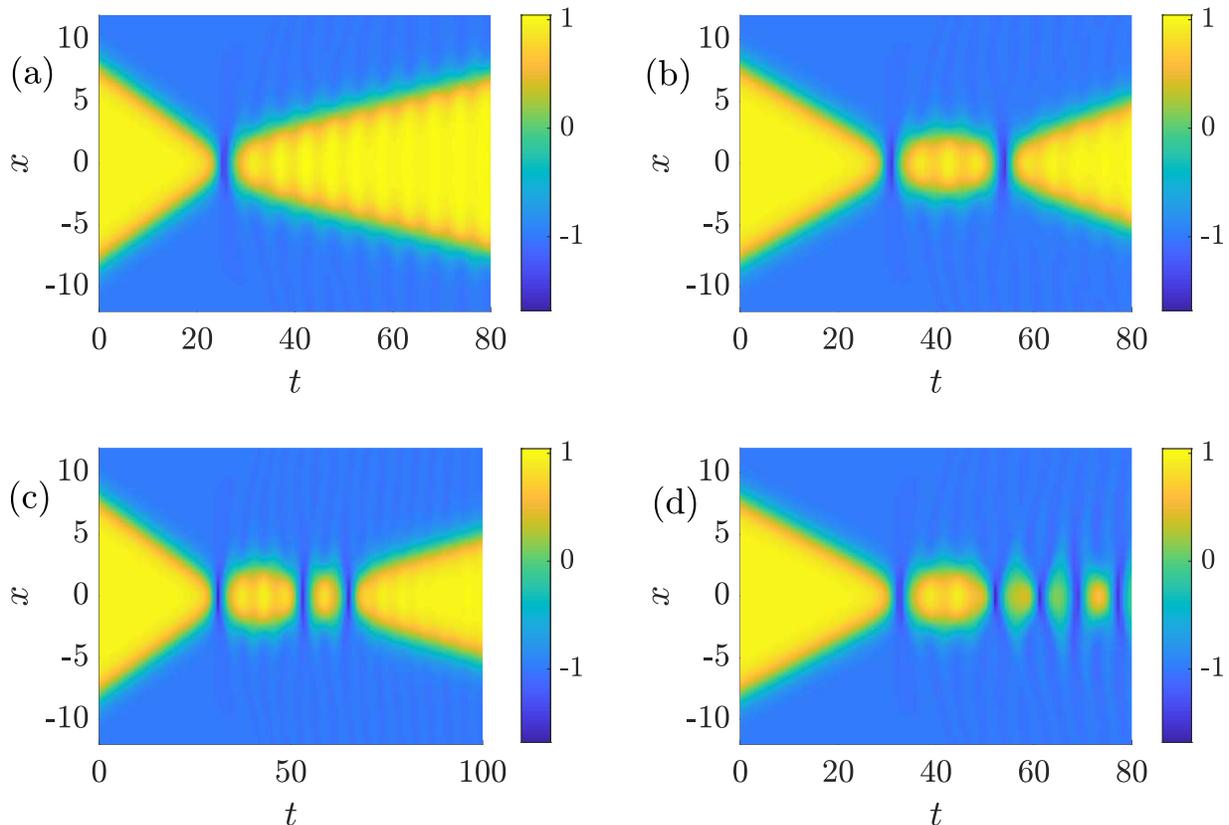


FIG. 2: Simulations of ϕ^4 kink-antikink solutions with varying initial velocity: (a) $v_0 = 0.28$, one-bounce solution, (b) $v_0 = 0.225$, a two bounce solution, (c) $v_0 = 0.2211$, a three-bounce solution, and (d) $v_0 = 0.21$, illustrating capture and bion formation.

IV. THE CURIOUS CASE OF THE ϕ^4 MODEL: COLLISIONS AND MULTI-BOUNCE WINDOWS

Based on the above section, it is tempting to think that the collision dynamics of non-integrable Klein-Gordon PDEs behave, up to small variations, just like their integrable counterparts. Compare the kink-antikink solutions for the sG system in Fig. 1(a) with the kink-antikink solution to ϕ^4 in Fig. 2(a), both given with a relatively large initial velocity $v = 0.28$. The two simulations seem roughly similar, but with a few nontrivial differences. First note that since $u = 2\pi m$ is a stable equilibrium of sG for all m , kinks and antikinks pass through each other following a collision, whereas in ϕ^4 , with only two stable equilibria, kinks and antikinks are reflected following a collision. One can also see that the sG kinks collide elastically: after the collision they pass through each other and continue with their original incoming speed. On the other hand, the ϕ^4 kinks bear the signature of the non-integrability of the model. In particular, their collisions are *inelastic* and as a result the kink and antikink lose kinetic energy in the collision, as is evident from the reduced slope in the space-time contour plot. A secondary effect is slightly harder to discern at first glance, but is all-important. Namely, after the collision, the kinks in the ϕ^4 simulation seem to be slightly “wobbly.” This, we will see momentarily, is due to an internal vibration of the coherent structures.

However, simulations of the ϕ^4 model with lower initial speeds result in *dramatic departures* from the elastic (irrespective of the kink speed) collisions seen in the integrable sG model. Fig. 2(b) and (c) show the results of collisions with $v = 0.225$ and $v = 0.2211$ respectively. These demonstrate, respectively, what are now known as a two-bounce solution, in which the kink and antikink collide, begin to separate and then re-collide before “escaping” each other’s attraction, and a three-bounce solution, which features one more round of separation and re-collision than the two-bounce solution. In fact, if the speeds of the waves are sufficiently low, then they are never able to escape each other’s attraction and persist in a long-lived trapped waveform which is termed a “bion”, as is shown in Fig. 2(d). The keen-eyed will observe the presence of radiation propagating ahead of the escaping kink-antikink pairs in all these images. Obviously, such features are unprecedented, and indeed impossible, in integrable systems.

In the late 1970’s and into the 1980’s, researchers became intrigued by the deviations between the dynamics in ϕ^4 and

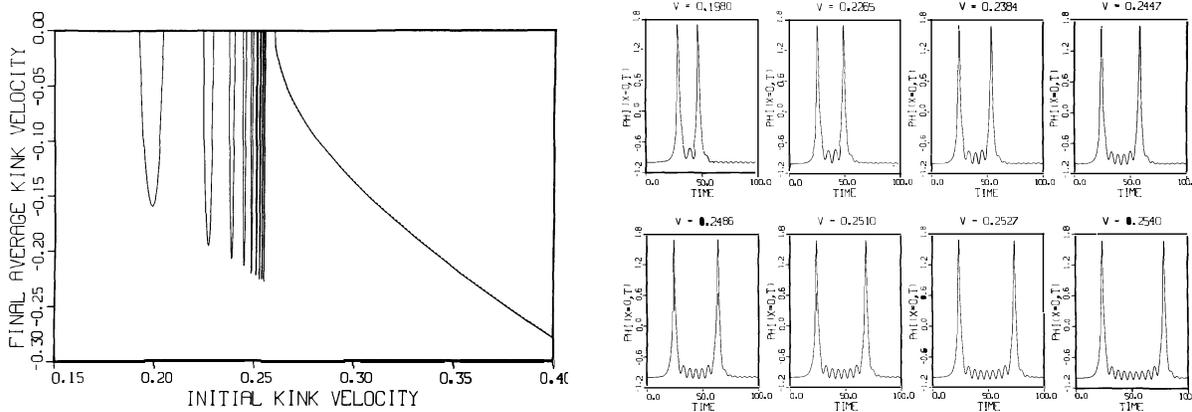


FIG. 3: Typical examples from the work of [11] as adapted in [31] (used with permission from the latter). The left panel shows the area of two-bounce windows of outgoing vs. incoming velocity, before the single-bounce occurring after the critical velocity of $v_c \approx 0.2598$. The right panel shows how progressively more vibrations of the internal mode occur when probing the field at the origin $u(0, t)$ as a function of time for select speeds in the different two-bounce windows.

related non-integrable models relative to those described by the IST for integrable systems and began to appreciate their relevance in mathematics and physics. Early numerical studies by numerous researchers—Kudryavtsev [33], Aubry [7], Getmanov [24], among others—reported the possibility of trapping, but arguably Ablowitz, Kruskal and Ladik [3] first reported the possibility of multi-bounce solutions. Numerical simulations back then were slow, expensive, and difficult to visualize. Each of these studies reported on a small handful of simulations.

The first to realize the complexity of these collisions were D. Campbell and his group at Los Alamos, who performed the first reasonably thorough numerical study, systematically tabulating the value of the outgoing collision velocity as a function of incoming collision velocity [11]. This is reproduced in the left panel of Fig 3. They found that at initial velocities above a critical value v_c , the kink and antikink escape after a single inelastic collision. Below this value, they found that the two-bounce solutions occur in a sequence of “windows” of finite width. At the center of each window is a “resonant velocity” at which the output speed nearly equals the input speed. They did not report any three-bounce solutions. The right panel shows the value of $u(0, t)$ for simulations of collisions at each of the resonant velocities. The two collisions occur at the large maxima, and each shows one more “bump” between the two collisions than the one before it. These simulations used so much computational resources that Campbell’s supervisor at Los Alamos, A. Scott, had to check in with him to make sure it was necessary [37]. D. Campbell has written a very accessible overview of these first efforts in the first Chapter of [31].

The key insight of [11] is that two-bounce windows are made possible due to the presence of an internal mode in the spectrum of the ϕ^4 kink. Indeed, the spectrum of the sG equation linearized around the sG kink consists solely of a pair of zero eigenvalues (corresponding to the kink’s translational invariance) and the continuous spectrum (associated with the background states between which the kink interpolates). However, in the ϕ^4 case, the corresponding linearization yields a Pöschl-Teller (i.e. sech^2) potential that has an additional bound state with frequency $\omega_s = \sqrt{3}$ and eigenfunction (for a static kink centered at x_0):

$$u = \sqrt{\frac{3}{2}} \tanh(x - x_0) \text{sech}(x - x_0). \quad (15)$$

The factor $\sqrt{\frac{3}{2}}$ is chosen to normalize the solution for convenience in a later calculation. This internal mode provides the system with the ability to store potential energy in a neighborhood of the kink. Hence, the main idea is:

- The incoming kinks have (kinetic) energy $K = \frac{M}{2} v_{\text{in}}^2$ where the mass of the solitary wave is given by (6). The kink and antikink induce a potential corresponding to their mutual attraction, as discussed in previous sections.
- Some of this energy, upon collision, is converted to potential (internal) energy of this vibrational mode.
- Between the emission of small amplitude radiation (after all, the origin of inelasticity of the collision in a non-integrable model; one of the miracles of integrable systems is that collisions generate no such radiation) and the depositing of energy partly in this internal mode, the kinks are left with low enough kinetic energy that they are *unable* to escape each other’s attraction.

- As a result they only separate to a maximal distance, and then return and re-collide.
- At the second collision, the exchange of energy may go in either direction and depends both on the amplitude of the oscillatory mode *and its phase*.
- If the phase of the oscillatory is such that it returns sufficient energy to the propagating mode for the kink and antikink to escape their mutual attraction, the process is called *resonant*.
- If the kink and antikink do not escape on the second bounce, they may escape due to resonance on a later one.
- Because each collision generates radiation, in addition to exchange between the potential and kinetic modes, with each collision, the probability of eventual escape decreases. If enough energy is converted to radiation, a bion state will form.

Subsequent numerical studies by Anninos et al. [6] and by Goodman and Haberman [26] showed the existence of additional narrower windows corresponding to three or more bounce resonances. A recomputation of Fig. 3, using more modern numerical methods, is given in Fig. 4, from Goodman's contribution to Ref. [31], showing all computed n -bounce windows up to $n = 5$.

The resonance condition posited by [11] was that the internal (shape) mode frequency ω_s and the interval T_2 between subsequent collisions needs to satisfy $\omega_s T_2 = 2n\pi + \delta$, where δ is some offset phase to be found by a fit. Such windows were found numerically for $3 \leq n \leq 10$. Using particle mechanics, the authors of [11] were able to connect T_2 with the difference between the kinetic energy and the critical kinetic energy for kink-antikink separation according to $T_2 \propto (v_c^2 - v_n^2)^{-\frac{1}{2}}$. This phenomenological approach finally led them to an empirical formula for the n th two-bounce window; see also the right panel of Fig. 3. The relevant formula reads:

$$v_n^2 = v_c^2 - \frac{\alpha}{(2\pi n + \delta)^2}, \quad (16)$$

where α is an additional parameter determined by fitting. This was found to agree remarkably well with the location of the first 10 two-bounce windows! It provides a phenomenological explanation why there are no windows with $n = 1$ or $n = 2$ as these would return a negative value of v_n^2 given the empirical values of α and δ . Importantly, subsequent work of Campbell and collaborators showed that other non-integrable models such as the modified sine-Gordon equation [36], the double sine-Gordon equation [10], and others featured a similar phenomenology.

V. A SIMPLIFYING APPROXIMATION AND A CRUCIAL MISTAKE

The approach of [11] is quite useful in unveiling the principal mechanism of the two-bounce resonance, yet it is rather phenomenological in that it depends on the numerically-determined parameters α and δ in Eq. (16). This indicates that it is based on an incomplete mathematical understanding of the problem. A more quantitative theoretical framework is needed to avoid such dependence on fitting. Fortunately, even before the publication of [11], Sugiyama [38] derived a simplified system of model equations that sought to provide such a framework. This framework has two advantages over Manton's computation, described in Sec. III: first, it makes no assumption of large separation, an assumption violated by the colliding pair, and, second, it takes into account the transfer of energy to the secondary mode (15). Sugiyama's approach has been at the heart of numerous inquiries into the two-bounce phenomenon over several decades [6, 8, 26, 28, 38].

Sugiyama used the so-called variational method to derive a finite dimensional system of ordinary differential equations modeling the kink-antikink interaction. The method is often attributed to Bondeson et al. [9], but this paper was submitted a mere three days before Sugiyama's so the origin of the idea remains (for us) cloudy. The method applies to PDE systems derived from a variational principle, meaning that the PDE arises as the Euler-Lagrange equations minimizing a certain action

$$A(u) = \int L(u; t) dt = \iint \mathcal{L}(u(x, t)) dx dt. \quad (17)$$

For example the nonlinear Klein-Gordon models (7) have a Lagrangian of the form

$$L = \int_{-\infty}^{\infty} \frac{1}{2} u_t^2 - \frac{1}{2} u_x^2 - V(u) dx. \quad (18)$$

The method is simple: assume that the solution depends on a finite number of time-dependent parameters $a_1(t), \dots, a_n(t)$

$$u(x, t) = U(x; a_1(t), \dots, a_n(t)). \quad (19)$$

Substituting this ansatz into Eq. (17), and integrating with respect to x yields a finite-dimensional Lagrangian whose Euler-Lagrange equations yield an ODE system for the evolution of the parameters $a_j(t)$. The method yields equations for the minimizer of the action among all functions in the multi-parameter family (19).

The fidelity of the resulting dynamics can be no better than the quality of the guess, which in turn depends on the modeler's understanding of the system. For example, one could try an ansatz involving only the translational mode. In that case, the variational *trial solution* will have the form:

$$u = u_K(x - X(t)) + u_{\bar{K}}(x + X(t)) - 1. \quad (20)$$

When this is substituted in the field Lagrangian of the ϕ^4 model, the effective Lagrangian and equation of motion take the form:

$$L(X, \dot{X}) = a_1(X)\dot{X}^2 - a_2(X) \Rightarrow \ddot{X} = -\frac{1}{2a_1} [a_1'(X)\dot{X}^2 + a_2'(X)]. \quad (21)$$

Here the quantities $a_{1,2}(X)$ denote suitable overlap integrals—e.g. it is straightforward to obtain that $a_1(X) = (1/2) \int_{-\infty}^{\infty} (u_K' - u_{\bar{K}}')^2 dx$, where the prime denotes the derivative with respect to the function's argument. Given that the single dynamical equation in Eq. (21) conserves energy, the kinks in this “highly constrained” reduction of the infinite-dimensional (PDE) dynamics can do nothing but collide elastically. Using this ansatz eliminates the need to assume the kink and antikink are well separated but provides too few degrees of freedom to allow the observed phenomena in the case of the ϕ^4 model.

We can achieve greater fidelity by including an internal mode in the ansatz. This permits an energy exchange between the total energy (kinetic plus potential) and the additional potential energy stored in the internal vibration around the kink. In this case, the trial solution reads

$$u = u_K(x - X(t)) + u_{\bar{K}}(x + X(t)) - 1 + [A(t)\chi(x + X) + B(t)\chi(x - X)] \quad (22)$$

leading to the far more complicated Lagrangian of the form:

$$L = a_1\dot{X}^2 - a_2(X) + a_{31}(\dot{A}^2 + \dot{B}^2) - a_4(A^2 + B^2) + a_{32}\dot{A}\dot{B} - a_{42}AB + a_5(A - B) + \dots \quad (23)$$

This Lagrangian only contains what are thought to be “essential terms” of interaction, assuming that the amplitude of the internal modes is small enough that higher powers of A and B can be neglected or are secondary to the (up to quadratic) powers considered herein. Indeed, the work of Weigel and his group [40–42] reports on these higher powers too for completeness.

The crucial error of the work of [38] already occurred at this level. The expression for a_5 should read:

$$a_5(X) = -3\pi\sqrt{\frac{3}{2}} [2 - 2\tanh^3(X) - 3\text{sech}^2(X) + \text{sech}^4(X)]. \quad (24)$$

However, Sugiyama must have inadvertently changed the \tanh^3 to \tanh^2 , which allows the bracketed term to be simplified to $-\text{sech}^2(X)\tanh^2(X)$. This, sadly, was the expression effectively used throughout the literature. In the work discussed below, the Lagrangian is simplified by assuming $A = -B$, equivalent to assuming that the solution lies on the invariant manifold of solutions satisfying even symmetry $u(x, t) = u(-x, t)$. That is, one can easily check that solutions to (23) with $A(0) = -B(0)$ and $\dot{A}(0) = -\dot{B}(0)$ satisfy $A(t) = -B(t)$ for all $t > 0$.

This mistake propagated from [38] to all the crucial works that followed considering the analysis of this model including, e.g., [6, 8, 26, 28]. Anninos et al. showed numerically that the two-degree of freedom ODE system possesses a fractal like structure, with three-bounce windows accumulating near the edges of the two-bounce windows, four-bounce windows at the edges of the three-bounce windows, etc; Fig 4(b).

Goodman and Haberman followed this up with a comprehensive analysis of Sugiyama's ODE system [27]. Using phase plane analysis, Melnikov integrals, and matched asymptotics expansions, they derived analytical expressions for the critical velocity v_c as well as the parameters α and δ given in equation (16) (without recourse to parameter fitting), as well as similar formulas for the locations of the three-bounce windows. Unfortunately, this analysis was performed on the ODE with the problematic a_5 term. Subsequently, they extended this analysis to reduce the ODE system to a discrete-time iterated map, for which they derived a detailed bifurcation diagram [25]. For purposes of

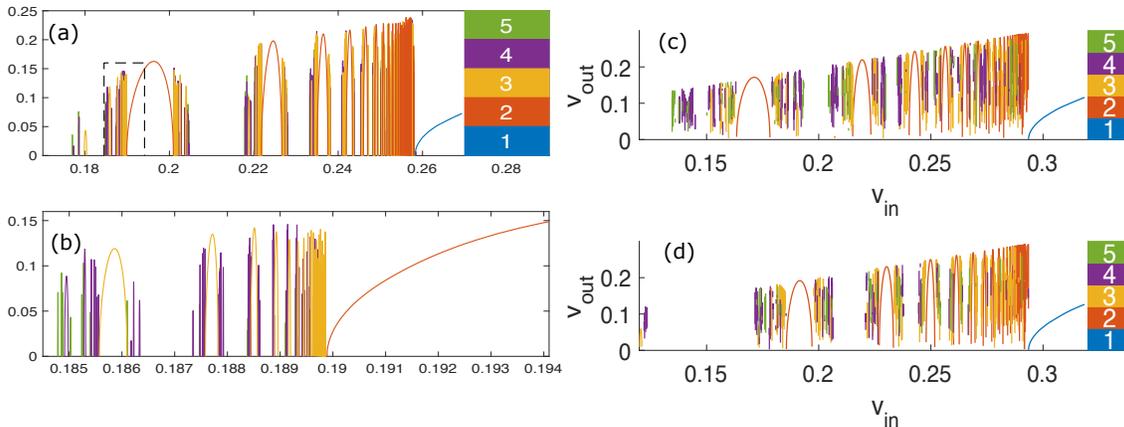


FIG. 4: Modern renderings of the results of Fig. 3 showing (a) results of PDE simulations, (b) zoomed-in view of the dashed box above it, demonstrating fractal-like structure, (c) equivalent image from the qualitative ODE model, (d) equivalent image generated by discrete map approximation to ODE model; adapted with permission from [31].

exposition, they worked in this paper with an idealized ODE model that retained the essential dynamical features of Sugiyama’s ODE system, while having a somewhat simpler structure. Such a map reproduces in great detail much of the fractal structure seen in the ODE model; see Fig 4(d).

In addition to noticing the problem with the a_5 term and correcting it, Weigel’s group pointed out that the qualitative and semi-quantitative match disappears when the corrected form of a_5 is used [40–42]. They further showed, to make matters worse, that the disagreement between ODE and PDE results only increases when higher order terms neglected in (23) are included. One final problem makes matters even gloomier, the so-called null-vector singularity. The internal mode (15) moves in a potential defined by the kink. However at $X = 0$ the term (20) representing the kink and antikink in the more general ansatz (22) vanishes, rendering the concept of an internal mode meaningless. This fact arises in the context of the evolution equations by making the mass matrix associated with the dynamical evolution singular when $X = 0$. Such a singularity is absent in the original PDE and is a mere side effect of the ODE reduction method; Caputo et al. recognized this problem in the early 1990’s and showed how to remove the singularity via a nonlinear change of variables [12, 13].

To avoid such issues, Weigel’s group [40–42] proposed the following modified ansatz in the variational trial function:

$$u = u_K(x - X) + u_{\bar{K}}(x + X) - \tanh(qX) + [A\chi(x + X) + B\chi(x - X)]. \quad (25)$$

This introduces a repulsive potential in the vicinity of $X \rightarrow 0$, which, in turn, precludes the kink and antikink from hitting the singularity at $X = 0$. Of course, this now adds an artificial potential and q becomes a tunable parameter which must be chosen optimally in order to optimize the fidelity of the reduced model to the original PDE. This can be done in a variety of ways, including selecting q to capture the right PDE outgoing velocity, or in order to capture the right number of bounces, or to possibly minimize the distance from the PDE kink-antikink center trajectory, or satisfy some other suitable cost function criterion. Whichever way is selected though cannot bypass the fact that this is a phenomenological and seemingly artificial inclusion that cannot be made systematic.

Remarkably, this suggests that despite a tremendous effort and 40 years of significant developments, we are still missing a quantitative understanding of the relevant phenomenology of what is arguably the simplest non-integrable collision dynamical model (the ϕ^4 model), in the context of the simplest type of coherent structures (heteroclinic, real-valued kinks with only one internal mode). We highlight this because the examples in the following section are more elaborate and have more complex and tunable features. This appears to be a disaster, but we choose, instead, to view it as an opportunity.

Clearly, we have amassed a tremendous amount of experience about the relevant phenomenology. The fractal-like structure of multi-bounce windows is well-established, and we know that it arises due to the (nearly) reversible transfer of energy between translational and vibrational modes. This is known to be due to the internal mode. Yet, we still lack a systematically-derived model that quantitatively characterizes this structure.

Perhaps a relevant suggestion in this direction is a beyond-two-mode ansatz that properly incorporates not only the translational and internal modes, but also the potential of the kink to radiate energy through modes of the continuous spectrum. This irreversible transfer to background modes is one of the significant features lacking in all of the earlier

considerations. A formal analysis including the leading-order effects was used to derive a nonlinear damping term in a similar variational model describing the interaction of a sine-Gordon with a delta-function potential in [29]. The effects of adding such a term to the variational model equations for the ϕ^4 model are discussed in [28].

A deeper question concerns the variational method itself. Despite its popularity in the mathematical physics literature going back at least 40 years, we know of only a single instance of a mathematical theorem proving that it works for any particular problem. That is, we know of only one paper in which an approximation derived using the variational method has been shown to remain close to the full solution of a PDE model over a time period of interest. In contrast to methods such as averaging or multiple scales, the variational approximation is not a perturbation method; it does not depend on a small parameter, so that applying the method does not yield an explicit remainder term which can afterward be shown small with respect to that parameter. By contrast, it is standard procedure to first apply a formal perturbation method such as averaging and to justify afterward it analytically. Chong et al. show that variational approximations to time-periodic orbits in a discrete NLS become increasingly accurate as a small parameter in that problem is reduced [14]. This result both depends on a small parameter and makes use of the time-periodicity of the solutions and thus does not generalize to the problem being discussed which is a general initial value problem with no small parameters. Chong’s work follows an earlier non-rigorous result due to Kaup and Vogel [30], which bounds the error due to the method but only to the special case of steady solutions, in which case the variational method yields algebraic equations. Therefore, we make a plea to our analyst colleagues: explain why and when the variational method works, or help us replace it with a justifiable method!

VI. RECENT DEVELOPMENTS: BEYOND THE ϕ^4 MODEL

In addition to recent developments in the ϕ^4 realm, the last decade has witnessed the discovery of intriguing features in higher-order models. One of the most well-established such models is the ϕ^6 equation, which arises in the work of Dorey *et al.* [22]. The potential in its Lagrangian (18) takes the form:

$$V(u) = -\frac{1}{2}u^2(u^2 - 1)^2. \quad (26)$$

The system possesses equi-energetic minima $u = -1, 0, 1$, as well as kink solutions that connect the various pairs of minima, such as,

$$u = \pm \sqrt{\frac{1 + \tanh(x)}{2}}, \quad (27)$$

and which can be Lorentz boosted to construct moving kinks. Remarkably, kink-antikink collisions in this model display resonance windows, despite the fact that the linearization about these kinks contains no internal modes: their only discrete eigenmodes correspond to the translation invariance of the underlying equations. These authors make the groundbreaking qualitative observation that, instead of considering the spectrum of an isolated kink, one must consider the spectrum of the linearization about the *dynamic configuration* of a kink-antikink pair moving towards each other. They find that this linearized system possesses a (transient) internal mode which they claim is responsible for the resonance phenomena. This is a bold proposal that requires some firm mathematical “backing”. It poses the more general question of the potential meaning of spectral features around a time-dependent state for which there is no frame where it can be considered stationary. In dissipative systems where the spectral gap may allow only for a few modes to be dynamically relevant, this may be easier to justify, but understanding the meaning of such a spectral analysis in Hamiltonian, conservative problems is a *wide open* field for future consideration.

Remarkably, this is not the only ϕ^6 model that has yielded new results. Demirkaya et al. [19] have recently considered a different ϕ^6 model proposed by Christ and Lee in 1975 (!) as a “bag model” where the domain walls (kinks) play the role of quarks within hadrons in high-energy physics [15]. They consider the potential:

$$V(u) = \frac{1}{8(1 + \epsilon^2)}(u^2 + \epsilon^2)(1 - u^2)^2. \quad (28)$$

Remarkably and despite its functional complexity, the model features an exact (static) kink solution:

$$u = \frac{\sinh\left(\frac{x}{2}\right)}{\sqrt{1 + \epsilon^{-2} + \sinh^2\left(\frac{x}{2}\right)}}. \quad (29)$$

Perhaps even more importantly, the linearization around this kink features a controllable number of internal vibrational modes, with a single mode in the $\epsilon \rightarrow \infty$ limit, where this model reduces to ϕ^4 , and an increasing number of modes,

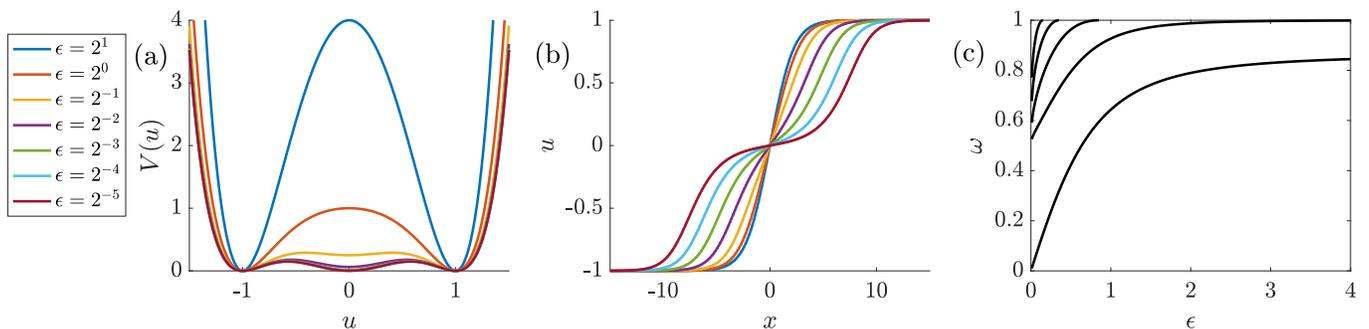


FIG. 5: Typical results from the ϕ^6 model of [19]. Legend shared by subplots (a-b). (a) The potential $V(u)$ for different values of ϵ —for larger ϵ it behaves like ϕ^4 , while as $\epsilon \searrow 0$ it approaches a triple well with three equal minima. (b) The corresponding kinks, approaching the tanh kink of ϕ^4 for large ϵ and approaching a two-step structure as ϵ decreases. (c) The discrete spectrum as a function of ϵ , showing two eigenvalues for large values of ϵ and additional eigenvalues bifurcating from the band edge at $\omega = 1$ as ϵ is decreased.

which is unbounded as $\epsilon \rightarrow 0$. The relevant potential, solitary waves and linearization features are shown in Fig. 5. The work of [19] showed that this ϕ^6 model possesses fewer multi-bounce windows as ϵ was decreased. This makes intuitive sense: a larger number of internal modes allows the energy to split into more pieces, making it less likely that on subsequent collisions, they will simultaneously return their energy to the propagating mode.

More recent studies have considered models involving higher order potentials, namely the ϕ^8 , ϕ^{10} and ϕ^{12} defined by

$$V(u) = u^{2n}(1 - u^2)^2,$$

for $n = 2, 3$, and 4 respectively. This is not just “more of the same”; such models hold substantial mathematical promise in their own right and are physically motivated by structural phase transitions in materials science [32]. Unlike previously-considered systems, they support *power law tails*. Since the kink stationary state satisfies: $\frac{du}{dx} = \sqrt{2V(u)}$, the following decay property calculation holds for the tails [17]. Suppose that as $x \rightarrow -\infty$, $u \rightarrow \bar{u}_i$ at algebraic rate k_i , and (respectively as $x \rightarrow \infty$, $u - u_{i+1} \sim x^{-k_{i+1}}$), then, letting

$$V(u) = (u - \bar{u}_i)^{k_i} (u - \bar{u}_{i+1})^{k_{i+1}} V_1(u), \quad (30)$$

$$\int dx = \int \frac{du}{(u - \bar{u}_i)^{k_i/2} (\bar{u}_{i+1} - u)^{k_{i+1}/2} \sqrt{2V_1(u)}}. \quad (31)$$

$$\int dx \approx \frac{1}{(\bar{u}_{i+1} - \bar{u}_i)^{k_{i+1}/2} \sqrt{2V_1(\bar{u}_i)}} \int \frac{du}{(u - \bar{u}_i)^{k_i/2}}. \quad (32)$$

Hence, e.g., for the ϕ^8 model, a kink connecting -1 and 0 has asymmetric tails of the form:

$$u_{(-1,0)}(x) \approx -\frac{1}{\sqrt{2}x}, \quad x \rightarrow +\infty; \quad (33)$$

$$u_{(-1,0)}(x) \approx -1 + \frac{2}{e^2} e^{2\sqrt{2}x}, \quad x \rightarrow -\infty. \quad (34)$$

and similarly for the kink between 0 and 1 .

This power law decay of the kink has numerous implications. A rather unexpected one arose in the attempt to explore collisions: a numerical initial condition consisting of a superposed a kink and an antikink with these fat tails, using either a sum or a product superposition, simply does not work. Fig. 6 shows the result of such a naive attempt: the numerics seems to suggest repulsion between the kink and antikink. Yet, that conclusion is in contrast with a theoretical calculation given below. It stems from the fact that the long-range tail of one of the structures dramatically modifies the field vicinity of the other, skewing the “true” interaction between the coherent structures in an undesirable way. The problem is that, because of the tails’ slow decay, the superposition of the two widely-spaced

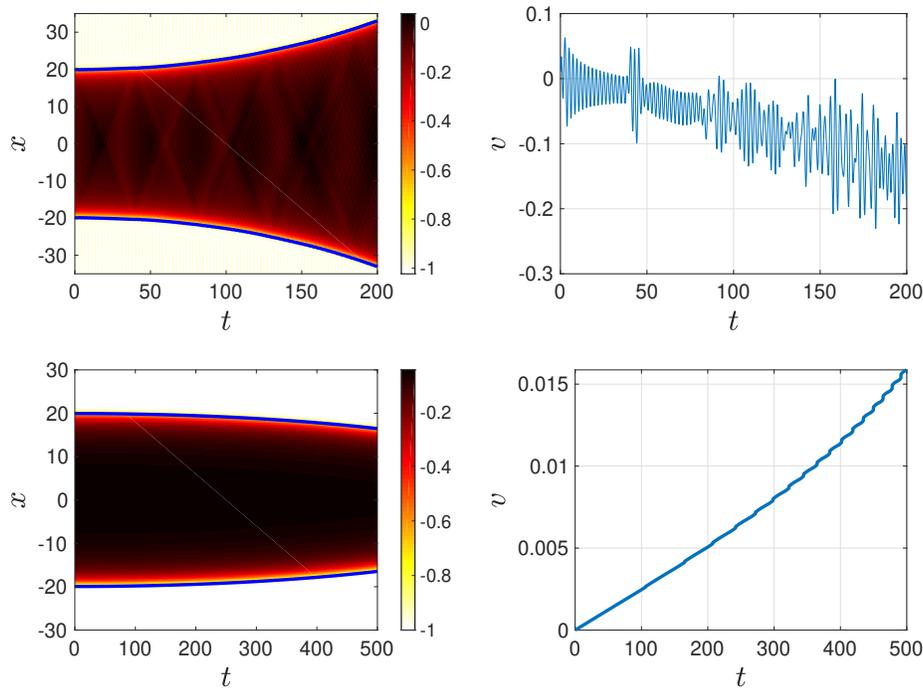


FIG. 6: The unexpected impact of fat tails in the ϕ^8 model: a sum ansatz incorrectly seems to lead to kink-antikink repulsion (and to a highly noisy velocity pattern) in the top panels. The bottom panel showcases the result of the “vacuuming” procedure (explained in the text) applied to the same ansatz, leading to a much less noisy (as inferred by the velocity evolution of the right panel) and indeed, as expected, attractive kink-antikink interaction. Adapted from [17].

and stationary solitary waves does not have small acceleration ϕ_{tt} at all points x . If instead, a minimization procedure is used to create an initial condition resembling such a superposition, but with ϕ_{tt} small everywhere, then the ensuing simulations do indeed produce the expected behavior. The bottom panel of Fig. 6 shows the dramatic impact of this procedure in unveiling the true, attractive nature of the interaction between a kink and an antikink in the ϕ^8 model, contrasting the apparent repulsion shown in the top panel.

Most recently, calculations in the past few months have characterized the kink-antikink and kink-kink asymptotic interactions in these higher order models. The acceleration of the kink-kink interaction as a function of their separation X was found to be given by:

$$a = \left[\frac{\Gamma(\frac{n-1}{2n})\Gamma(\frac{1}{2n})}{2n\sqrt{\pi}} \right]^{\frac{2n}{n-1}} \frac{(n+1)(n+3)}{4} X^{\frac{2n}{1-n}}. \quad (35)$$

while the acceleration of a kink-antikink pair is given by:

$$a = \left[\frac{-\sqrt{\pi}\Gamma(\frac{n-1}{2n})}{\Gamma(-\frac{1}{2n})} \right]^{\frac{2n}{n-1}} \frac{(n+1)(n+3)}{4} X^{\frac{2n}{1-n}}. \quad (36)$$

These findings [16, 35] were recently compared with numerical computations yielding very good agreement both for the kink-antikink and for the kink-kink interactions; see Fig. 7.

VII. THE PATH FORWARD: OPPORTUNITIES AHEAD!

So, where does this all leave us? Integrable systems are, of course, well understood. For non-integrable models, the “flagship” problem of the ϕ^4 model still lays mathematically wide open! We have a good sense of what is going on—resonant transfer of energy from the propagating mode to an internal mode during the initial collision, and further exchange of the energy on later collisions lead to the fancy fractal multi-bounce windows. Yet, after 40 years, we currently have no satisfactory proof or quantitative characterization of the phenomenon.

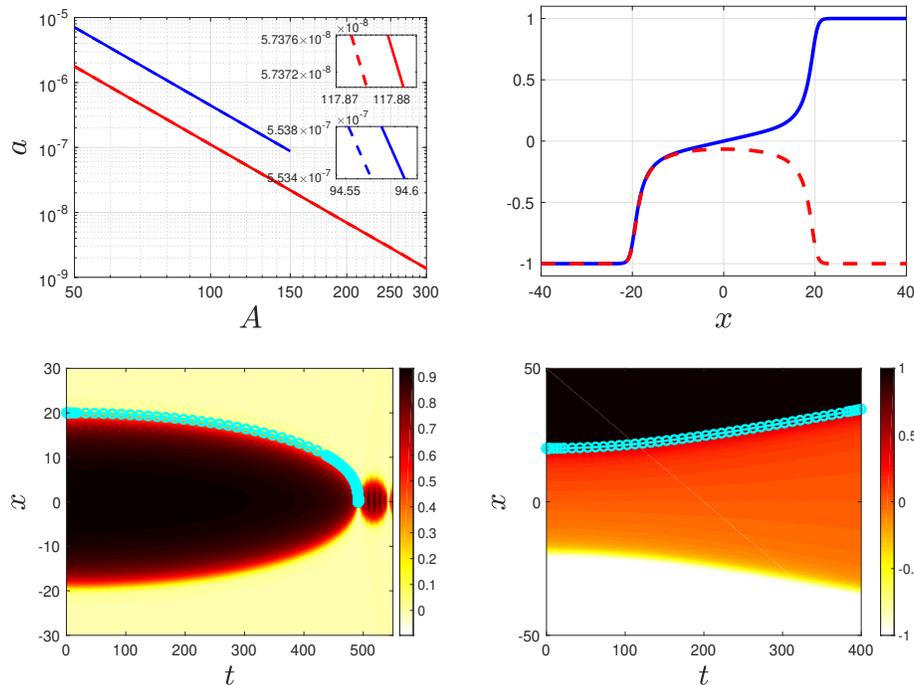


FIG. 7: (Top left) Kink-antikink (red) and kink-kink (blue) acceleration as a function of their separation. Inset shows the theoretical and numerical computations to be indistinguishable. (Top right) Typical corresponding spatial profiles for the kink-antikink (dashed red) and the kink-kink (solid blue). (Bottom left) A kink-antikink simulation, displaying attraction. (Bottom right) A kink-kink simulation, displaying repulsion. The circle symbols denote the results of the corresponding one degree-of-freedom ODE reduction. The relevant results have been obtained recently in [16].

Then, there is a whole other world of Klein-Gordon models with higher-order nonlinearities. The next challenge is the ϕ^6 model. It seems as if transient spectra and internal modes thereof are dynamically relevant. But it is unclear how to understand this in a mathematically convincing way. Another intriguing situation concerns systems that have not one, but two or many internal modes, as is controllably possible here. What happens to the resonance picture in this setting?

Higher order models offer another significant stepping stone. Here, the exponential decay (and its nice superposition properties due to the kinks' fast decay) are out the window. This has important implications for numerical simulations, where initial conditions must be chosen judiciously in order to avoid spurious effects. What are the implications of all this for the collisions and the resonance mechanisms? Are there internal modes in this case, and if so, what role do they play? Also, these systems possess asymmetric kinks with, on their two ends, exponential and power law decay. Can we induce some sort of competition between a shorter distance but exponentially decaying tail effect and a longer distance but fat (power law) tail effect? All these remain wide open questions in a theme that is just starting to warm up.

It is amusing to think that kink collision numerical experiments started very early on in the history of solitonic dynamics. Yet, some four (and a half) decades later, they remain as challenging, as they appear (deceptively) simple. It seems that there are a few (or a lot) more kinks to iron out before the story is complete!

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