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Kink–Antikink Scattering in φ^4 and ϕ^6 Models

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Abstract. For kink–antikink scattering within the φ^4 non–linear field theory in one space and one time dimension resonance type configurations emerge when the relative velocity between kink and antikink falls below a critical value. It has been conjectured that the vibrational excitation of the kink would be the source for these resonances because (simplified) collective coordinate calculations, that emphasized on this excitation, qualitatively reproduced those resonances. Surprisingly a numerical study in the ϕ^6 field theory also exhibited such resonances even though it does not contain the vibrational excitation. To explore this contradiction we start from the working hypothesis that in either model any collective coordinate ansatz which includes a degree of freedom similar to the vibrational excitation leads to resonances, regardless of whether or not this mode emerges as a solution to the (linearized) field equations. To this end we compare numerical results in the φ^4 and ϕ^6 models that arise from the full set of partial differential equations to those from the ordinary differential equations for a collective coordinate ansatz. An inaccuracy in literature formulas for the collective coordinate approach in the φ^4 model requires to revisit those calculations.

1. Motivation

The kink soliton in the φ^4 model is often considered as the prototype [1] configuration for more elaborate soliton systems that occur in field theory. The range of physics disciplines in which solitons are relevant is huge. Solitons appear in cosmology [2,3], particle and nuclear physics [4,5], as well as condensed matter physics [6]. Kink–antikink configurations are of particular interest because they can mimic particle–antiparticle interactions and might eventually provide more inside into fundamental concepts like crossing–symmetry in particle scattering [7]. Using modern desktop computers, numerical solutions to the field equations that initially represent a widely separated but approaching kink–antikink pair are feasible. This amounts to numerically integrating partial differential equations (PDE) for time and space dependent fields. Nevertheless it is interesting to simplify those equations by assuming collective coordinate ansätze. This reduces the PDE to coupled ordinary differential equations (ODE) for a limited number of time dependent functions. Equally interesting, collective coordinates may also answer the question of which are important modes of the system. In this context, the so–called *shape mode* in the φ^4 model has attracted particular attention. This mode is a bound state in the vibration spectrum about the kink [8]. It has been assumed to be responsible for the *bounce* type solutions to the PDE in kink–antikink interactions [9]. These bounce solutions are resonating kink–antikink configurations. The perception is that the shape mode can absorb sufficient energy from the kink–antikink system to prevent it from falling apart after collision. This role of the shape mode has been doubted as the ϕ^6 model also contains bounce type solutions in the kink–antikink sector(s) [10]. However, apart from the translational zero mode there is no bound state in the vibration spectrum of the kink in the ϕ^6 model. In this model thus a thorough investigation of the collective coordinate analysis is required to better understand this contradiction. We will do so in sections four and five and adopt the working hypothesis that a collective coordinate ansatz with a shape mode type component will be a suitable approximation in either case. Furthermore it has turned out that the collective coordinate calculations in the φ^4 model have inherited (typographical) errors in the formula for the source term of the shape mode from ref. [11]. We will therefore revisit those calculations in section three. In all cases we will compare results from the corresponding ODE to solutions of the PDE, the full field equations. The latter are obtained with programming code adapted from that used in ref. [12]. We conclude and comment on the relevance of collective coordinate calculations in section six. We will, however, commence with a brief review of kink–antikink approaches.

2. Kink–Antikink Concept

By now there have been many detailed numerical studies [9, 13–16] of the PDE for the field in the φ^4 model in one time and one space dimension[1]. The model is defined by the Lagrangian

$$\mathcal{L}_4 = \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{1}{2}\left(\varphi^2 - 1\right)^2 , \tag{1}$$

where all model parameters have been absorbed by appropriate redefinitions of the coordinates (t, x) and the field φ. The field equation reads

$$\ddot{\varphi} - \varphi'' = 2\varphi\left(1 - \varphi^2\right) , \tag{2}$$

where dots and primes denote time and coordinate derivatives, respectively. The (anti)kink $\varphi_{K,\overline{K}} = \pm\tanh(x)$ is a static solution to this equation. It connects the two vacuum solutions at $\varphi_{\rm vac} = \pm1$. Kink–antikink configurations

$$\varphi_{K\overline{K}}(x, X(t)) = \varphi_K(\xi_+) + \varphi_{\overline{K}}(\xi_-) - 1 = \tanh(\xi_+) - \tanh(\xi_-) - 1 \tag{3}$$

with

$$\xi_\pm = \frac{x}{\sqrt{1 - v_{\rm in}^2}} \pm X(t) \qquad \text{and} \qquad \dot{X}(0) = \frac{-v_{\rm in}}{\sqrt{1 - v_{\rm in}^2}} \tag{4}$$

are solutions for wide separation $X(t) \gg 0$. For these conventions $X(t)$ essentially measures the position of the antikink. More interestingly these configurations may serve as initial conditions for the equation of motion by choosing $X(0)$ large enough to avoid interference and the constant velocity $v_{\rm in}$ such that kink and antikink approach each other. A typical solution is shown in figure 1. The most interesting feature is the appearance of bounces for initial velocity $v_{\rm in}$ below a critical value $v_{\rm cr}$. The example in figure 1 has two bounces but solutions with many bounces (and traps) exist too [9]. The occurrence of such bounces has frequently been linked to the existence of the so–called shape mode

$$\chi(x, t) = {\rm e}^{i\omega_1 t}\chi_1(x) \qquad \text{with} \qquad \chi_1(x) = \frac{\sinh(x)}{\cosh^2(x)} \tag{5}$$

with eigen–frequency $\omega_1^2 = 3$ in the vibration spectrum of the kink [8]. (The continuum spectrum starts at $\omega^2 = 4$ for the present units.) The common argument is that the collective coordinate parameterization

$$\varphi_{\rm cc}(x, t) = \varphi_{K\overline{K}}(x, X(t)) + \sqrt{\tfrac{3}{2}}\,A(t)\left[\chi_1(x + X(t)) - \chi_1(x - X(t))\right] , \tag{6}$$

[1] See ref. [9] for a comprehensive summary of these computations.

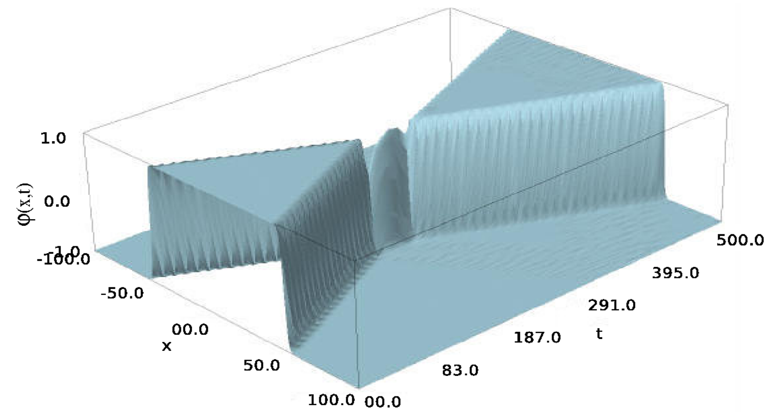


Figure 1. A typical solution to the PDE with kink–antikink initial conditions. Figure adopted from ref. [7].

that reduces the PDE (2) to the (simpler) ODE for the time dependent collective coordinates $A(t)$ and $X(t)$, not only approximates the full solution reasonably well, but also reproduces $v_{\rm cr}$ within 10% [9][2]. In the above ansatz the difference of the shape modes at $\xi_\pm$ is assumed because the (anti)kinks do not directly excite the sum.

Similar bounces and traps have been recently observed [10] in the ϕ^6 model which is defined by the Lagrangian

$$\mathcal{L}_6 = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}\phi^2\left(\phi^2-1\right)^2 \,. \tag{7}$$

Although the corresponding field equation

$$\ddot{\phi} - \phi'' = -\phi\left(3\phi^4 - 4\phi^2 + 1\right) \,, \tag{8}$$

also allows for (anti)kink solutions $\phi_{K,\overline{K}} = [1+\exp(\pm 2x)]^{-\frac{1}{2}}$, there is no bound state with non–zero energy in the vibration spectrum about the kink. This suggests that the existence of the shape mode does not serve as a rigorous criterion for the occurrence of bounces and traps.

In view of the above observed puzzle we reverse that line of argument into a working hypothesis. We want to test the assumption that the solutions of the ODE for the collective coordinate ansätze reasonably well approximate the solutions to the full PDE; regardless of whether or not $\chi(x,t)$ solves the field equation for vibrations in the kink background. For the φ^4 model the ansatz is given in eq. (6). There are two analogs in the ϕ^6 model

$$\begin{aligned}
\phi_{\rm cc}(x,t) &= \phi_K(\xi_+) + \phi_{\overline{K}}(\xi_-) + \sqrt{\tfrac{3}{2}}\,A(t)\left[\chi_1(x+X(t)) - \chi_1(x-X(t))\right] \,, &(9)\\
\overline{\phi}_{\rm cc}(x,t) &= \phi_K(\xi_-) + \phi_{\overline{K}}(\xi_+) - 1 + \sqrt{\tfrac{3}{2}}\,A(t)\left[\chi_1(x+X(t)) - \chi_1(x-X(t))\right] \,, &(10)
\end{aligned}$$

since there are three possible vacuum solutions, $\phi_{\rm vac} = 0, \pm 1$. We substitute these ansätze into the Lagrangian and integrate over the spatial degree of freedom. Formally the resulting Lagrangian for the collective coordinates reads

$$L_6(A,\dot{A},X,\dot{X}) = \int dx\, \mathcal{L}_6(\varphi_{\rm cc})$$

[2] Another argument is based on the perturbed sine–Gordon model [17].

$$= a_1\dot{X}^2 - a_2 + a_3\dot{A}^2 - a_4A^2 + a_5A + a_6\dot{X}^2A + a_7\dot{X}\dot{A}$$
$$+a_8\dot{X}^2A^2 + a_9A\dot{X}\dot{A} - a_{10}A^3 - a_{11}A^4 - a_{12}A^5 - a_{13}A^6\,. \tag{11}$$

The coefficient functions depend on the (relative) distance parameter, *i.e.* $a_i = a_i(X)$ for $i = 1, \dots, 13$. They also have a parametrical dependence on the initial velocity $v_{\rm in}$ via the construction in eq. (4). The φ^4 model has a similar collective coordinate Lagrangian, just that a_{12} and a_{13} are absent. The actual form of the a_i, of course, depends on whether eq. (9), eq. (10) or the φ^4 model is considered. As an example, we list

$$a_1(X) = \frac{1}{2}\int_{-\infty}^{\infty} dx \left[\mathrm{e}^{2\xi_+}\left(1+\mathrm{e}^{2\xi_+}\right)^{-\frac{3}{2}} + \mathrm{e}^{-2\xi_-}\left(1+\mathrm{e}^{-2\xi_-}\right)^{-\frac{3}{2}}\right] \tag{12}$$

for the system of eq. (9) in the ϕ^6 model. It is straightforward to compute these coefficients numerically for any prescribed value of X. This is completely sufficient for the subsequent numerical integration of the ODE for $X(t)$ and $A(t)$ that follow from the variational principle for the collective coordinate Lagrangians. For the φ^4 model analytic expressions for some of the coefficients have been derived some time ago [11, 14]. Unfortunately, the formulas presented in ref. [11] contain some misprints which propagated through the literature and make the quoted numerical results for the collective coordinate approach in the φ^4 model unreliable. We therefore revisit those calculations in the next section. The subsequent sections contain novel studies on the collective coordinate approach in the ϕ^6 model.

3. Revisiting the φ^4 model

The most impressive result from the collective coordinate approach in the φ^4 model is the prediction for the critical velocity $v_{\rm cr} \approx 0.289$ [9] above which bounces and traps cease to exist. This is only about 10% off from the exact result from the PDE, 0.26 [14]. However, a number of (uncontrollable) approximations to the system were used: All non–harmonic terms were omitted ($a_{10}, \dots, a_{13} = 0$), the ODE were diagonalized ($a_6, \dots, a_9 = 0$) and the direct interactions between the shape modes at $\pm X(t)$ were discarded via $a_i \mapsto \lim_{X\to\infty} a_i(X)$ for $i = 3, 4$ [16]. The latter approximation also avoids the null–vector problem discussed in ref. [18]

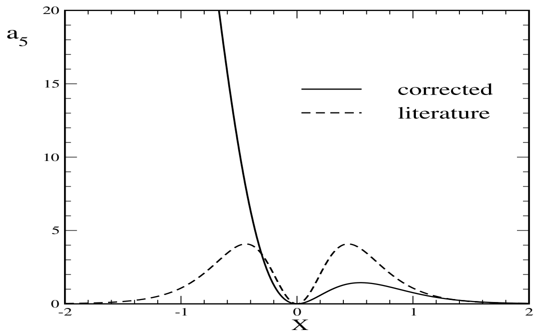
The source term for the shape mode, a_5 is interesting because it represents a small amplitude variation about the kink–antikink configuration. It should hence vanish only when $\varphi_{K\overline{K}}$ is a static solution to the field equation. To gain some insight into the form of a_5 before computing it explicitly it is instructive to consider

$$\varphi_{K\overline{K}}(0, X) = 2\tanh(X) - 1 \longrightarrow \begin{cases} 1 & \text{for} \quad X \to +\infty \\ -3 & \text{for} \quad X \to -\infty\,. \end{cases} \tag{13}$$

The second case suggests that $\varphi_{K\overline{K}}(x, -\infty)$ is not a solution to the field equations because then the center between widely separated kink and antikink profiles is not a vacuum configuration. But $\varphi(x, +\infty)$ is a valid solution. Hence, a_5 cannot be symmetric under $X \to -X$. However, that symmetry is erroneously reflected by the expression in the appendix of ref. [11], wherein it is called $F(X)$. Unfortunately, this incorrect expression has been used in all subsequent studies of the ODE. Redoing the calculation shows that the correct result is (for $v_{\rm in} = 0$)

$$a_5(X) = 3\sqrt{6}\pi\left[2 - 2\tanh^3(X) - \frac{3}{\cosh^2(X)} + \frac{1}{\cosh^4(X)}\right], \tag{14}$$

which obviously is not symmetric under $X \to -X$. Changing the power of the $\tanh(X)$ term from 3 to 2 and doubling the arguments of all hypergeometric functions reproduces the expression



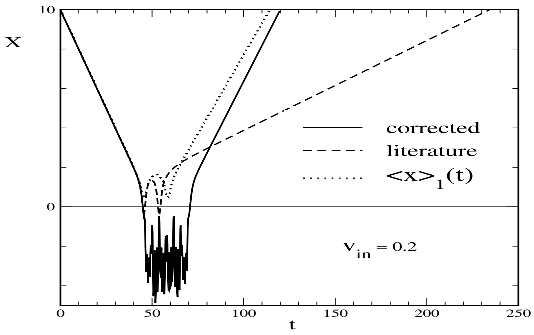


Figure 2. Left panel: Correction of the coefficient function $a_5(X)$ for $v_{\rm in} = 0$ (*corrected* refers to eq. (14), *literature* denotes the expression derived in ref. [11] and frequently adopted thereafter). Right panel: comparison of the resulting time dependence of the collective coordinate $X(t)$; the dotted line stems from the PDE with $n = 1$ in eq. (16).

in ref. [11]. In figure 2 the consequences of correcting this coefficient function are studied. As discussed above, the invariance of a_5 under reflection is lost. More importantly the solutions to the Euler–Lagrange equations for $X(t)$ and $A(t)$ that we solve for the initial conditions[3]

$$X(0) \to \infty\,, \quad \dot{X}(0) = \frac{-v_{\rm in}}{\sqrt{1-v_{\rm in}^2}}\,, \quad A(0) = 0 \quad \text{and} \quad \dot{A}(0) = 0\,, \tag{15}$$

change drastically when corresponding initial conditions and all of the above listed approximations are imposed. In figure 2 this is exemplified for the kink–antikink distance for the initial relative velocity $v_{\rm in} = 0.2$. Most notably, once the correction is installed, multiple bounces occur at any initial velocity.

A main intention is to quantitatively compare the solutions to the ODE to those of the PDE for the full field equation. We therefore estimate the time–dependent position of the the antikink as the expectation value

$$\langle x\rangle_n(t) = \frac{\int_0^\infty dx\, x\, \epsilon_4^n(t,x)}{\int_0^\infty dx\, \epsilon_4^n(t,x)}\,. \tag{16}$$

Here

$$\epsilon_4(t,x) = \frac{1}{2}\left[\ddot{\varphi} + \varphi'' + \left(\varphi^2-1\right)^2\right] \tag{17}$$

is the energy density for the solution $\varphi = \varphi(x,t)$ to the PDE (2) for initial configurations described by equation (6) at $t = 0$. The integer n can be freely chosen to eventually emphasize effects. Since the energy density is typically strongly localized, increasing n turns the distribution against which x is tested, into a δ–function. From the right panel of figure 2 we also see that the corrected ODE result shows almost no resemblance with the PDE solution, while the literature (though incorrect) one correctly reproduces the number of bounces. However, with the correction for a_5 installed the out–going velocity is well reproduced.

In view of these results we must question the above listed approximations. This is even more the case as the consistency conditions emerging from $\varphi_{K\overline{K}}(x,\infty)$ being a solution for $v_{\rm in} \neq 0$ read[4]

$$\lim_{X\to\infty}\left[a_5(X) + a_6(X)\,\dot{X}^2(0)\right] = 0 \qquad \text{and} \qquad \lim_{X\to\infty} a_7(X) = 0 \tag{18}$$

[3] Numerically we find that $X(0) \sim 10$ is an adequate representation of infinity as no overlap between the initial structures occurs.

[4] We have verified them both analytically and numerically.

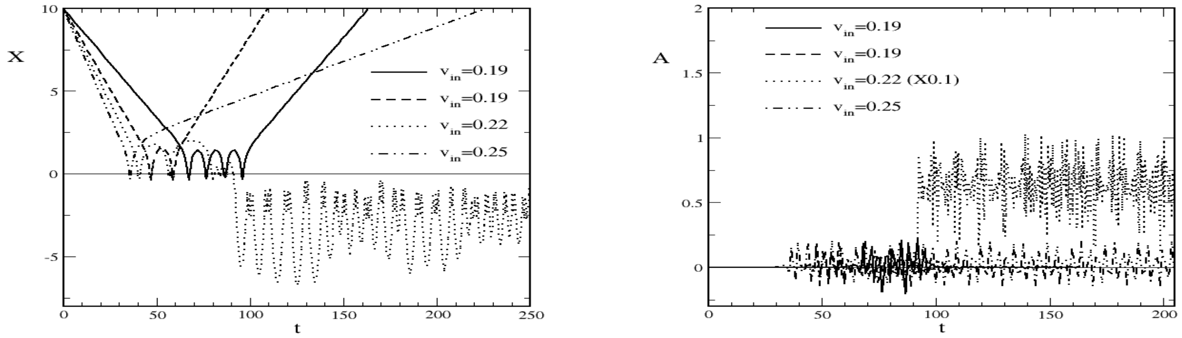


Figure 3. Solution to the ODE in the φ^4 model. Left panel: kink–antikink separation, right panel: amplitude of shape mode (note the change of scale in the $v_{\rm in} = 0.22$ entry).

and thus prohibit the omission of a_6. We have numerically solved the ODE for $X(t)$ and $A(t)$ with the sole approximation being that on $a_{3,4}$ to avoid the null–vector problem. (We comment on possible improvements in the summary section.). The results of these calculations are shown in figure 3. It turns out that with the correction on a_5, the corresponding contribution to the energy, $E_5 = -a_5(X)A$ may absorb much energy when X becomes negative. Hence trapping type solutions with large amplitudes of the shape mode emerge. A posteriori, this again disqualifies the harmonic approximation. The entry with $v_{\rm in} = 0.22$ in figure 3 is a typical example thereof. Most notably, however, we find that without the many approximations, the ODE indeed predict a critical velocity of $v_{\rm cr} = 0.247$ above which trapping or bounce type solution cease to exist. This compares favorably to the PDE result of 0.26 [14].

4. Antikink–Kink in ϕ^6

In the ϕ^6 model there are two types of initial structures that contain kink and antikink configurations. We first consider the so–called *antikink–kink* ansatz [10] of eq. (9) that, as in the φ^4 model, eq. (3), parameterizes a legitimate solution only for $X \to \infty$ but not for $X \to -\infty$. Hence it cannot describe penetration either. To compare the solutions to the ODE to those of the PDE for the full field equation in the ϕ^6 model we need to replace the energy density in eq. (16) by

$$\epsilon_6(t,x) = \frac{1}{2}\left[\ddot{\phi} + \phi'' + \phi^2\left(\phi^2 - 1\right)^2\right]. \qquad (19)$$

Here $\phi = \phi(x,t)$ are the solutions to the PDE (8) with initial conditions taken as the $t = 0$ configuration in eq. (9).

The PDE yields a critical velocity of $v_{\rm cr,PDE} = 0.05$ above which no traps or bounces occur. As shown in figure 4 the solutions to the ODE and PDE differ substantially at low initial velocities. Typically the bounce frequency from the ODE is much larger. So is the predicted critical velocity $v_{\rm cr,ODE} = 0.357$. It is thus suggestive that the collective coordinate approach over–estimates the attraction between kink and antikink. For velocities above $v_{\rm cr,ODE}$ this can also be observed as the ODE prediction for the final velocity is lower than that from the PDE. In the close vicinity of that critical velocity the technical parameters that enter the numerical treatment of the ODE seem to matter, thereby indicating chaotic behavior. In particular, the results are sensitive to the coordinate value that is supposed to represent infinity; as can be seen from the $v_{\rm in} = 0.35$ entry.

For large initial velocities the PDE results actually exhibit some pseudo–bounces shown in figure 5. The kink and antikink linger on top of each other for a moderate time interval. If the

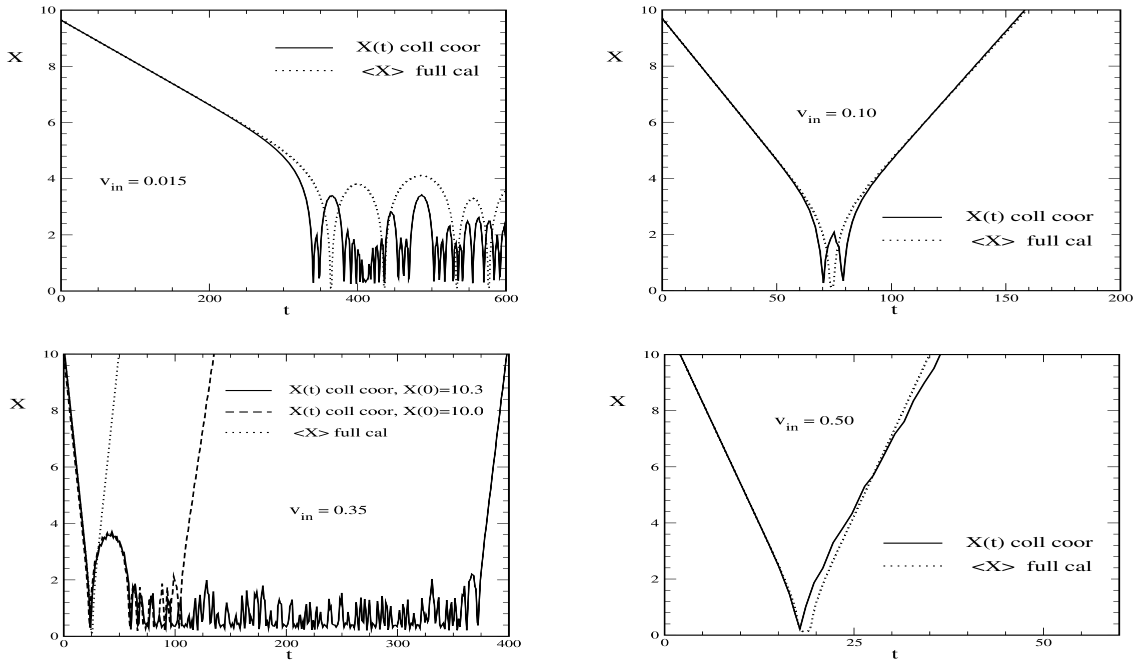


Figure 4. Solutions to the ODE for antikink–kink scattering in the ϕ^6 model and comparison to PDE results (*full cal*) with $n = 1$ in eqs. (16) and (19).

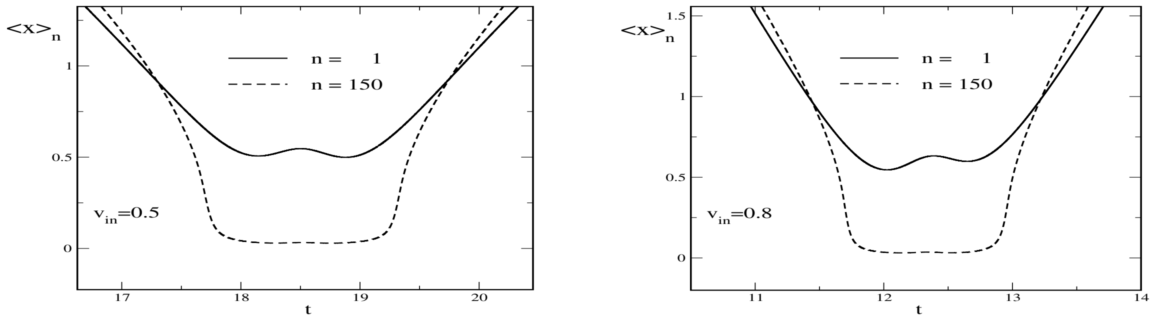


Figure 5. Pseudo–bounces in the antikink–kink system of the ϕ^6 model from the PDE . The parameter n enters the computation the expectation value of the position of the antikink via eq. (16).

distribution in eq. (16) is taken to be broad, the trajectory feigns mini–bounces.

5. Kink–Antikink in ϕ^6

In contrast to the previously discussed configurations the so–called *kink–antikink* structure from eq. (10) has topological properties which would allow it to be a solution even in the case $X \to -\infty$. However, the potential a_2 in eq. (11) is not symmetric under $X \to -X$ and $a_2(-\infty) > a_2(\infty)$. Hence there is a velocity threshold for solutions that correspond to the kink penetrating the antikink. Simple kinematical considerations on the ODE coefficients a_i indicate this threshold to be $v_{\rm th} = 0.296$. The numerical solution to the ODE yields a slightly larger value, 0.302. The left panel in figure 6 shows that the configuration with initial velocity $v_{\rm in} = 0.30$ bounces while bigger values of $v_{\rm in}$ yield $X(t) \to -\infty$ at large times. The ODE yields a window $0.216 \le v_{\rm in} \le 0.302$ in which the system bounces exactly twice. As for the φ^4 model,

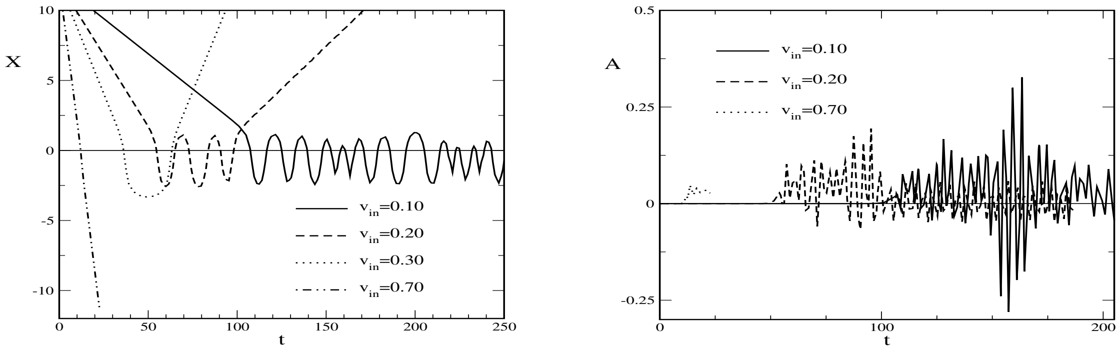


Figure 6. Solutions for kink–antikink interactions from the ODE system in the ϕ^6 model. Left panel: kink–antikink separation, right panel: amplitude of shape mode.

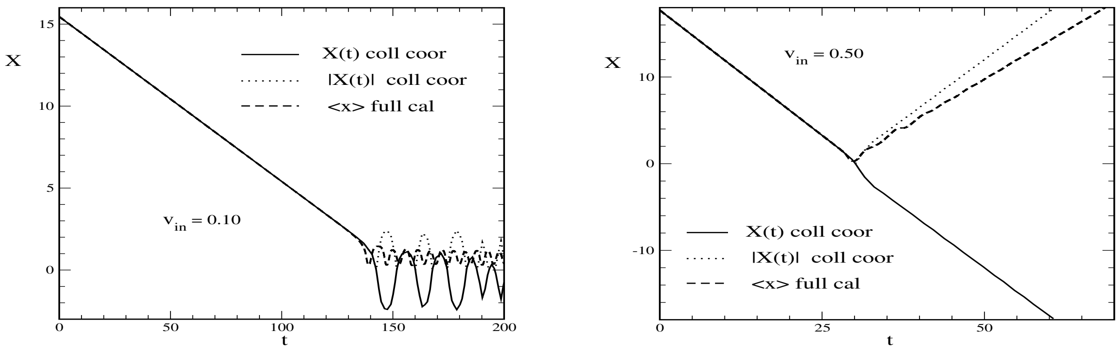


Figure 7. Comparison of PDE and ODE solutions for kink–antikink interactions in the ϕ^6 model. *Full cal* refers to $\langle x \rangle_1$ in eqs. (16) and (19).

multiple bounce solutions are characterized by a sizable amplitude of the shape mode. Even though this is not a valid vibrational solution it supports the working hypothesis that, once the collective coordinate ansatz allows for its excitation, it will do so. It should also be noted that the upper bound of the above mentioned window agrees reasonably well (but not perfectly) with the critical velocity (0.289) from the PDE calculation.

For $v_{\rm in} = 0.10$ and $v_{\rm in} = 0.50$ we compare the PDE and ODE results for the distances between kink and antikink figure 7. The PDE calculation for $\langle x \rangle$ is as in eqs. (8), (16) and (19). However, the initial condition at $t = 0$ is now taken from eq. (10). The structure within ODE and PDE solutions agree. However, if applicable, the frequency of bounces differs considerably.

6. Summary

Collective coordinate calculations are quite useful in non–linear field theory not only because they simplify the field equations considerably but also because they potentially provide insight into the underlying dynamics by focusing on particular modes. Within the φ^4 and ϕ^6 models in one time and one space dimension we have compared the ODE solutions from the collective coordinate approaches to those from the PDE for the space–time dependent fields. Our analysis, however, has revealed that care in needed when attempting to draw rigorous conclusions from collective coordinate calculations. Not only do they depend on the specific ansätze but also on the approximations made. For example, the harmonic approximation in the φ^4 model incorrectly yields solutions with repeated bounces for any relative initial velocity of the kink–antikink configuration (after correcting a literature error within the collective coordinate Lagrangian).

On the other hand the PDE yields quite a small critical velocity beyond which multiple bounces cease to exist.

Our studies support the working hypothesis that a shape mode in the vibration spectrum of the kink is not a necessity for bounces and traps to occur in kink–antikink scattering. We started from the conjecture that a collective coordinate ansatz including such a mode would represent the full field configuration reasonably well regardless of whether or not it is a true bound state of the kink. We have explored the (dis)agreements between the ODE and PDE results. These (dis)agreements are qualitatively equal in the φ^4 and ϕ^6 models. Since the shape mode only exists within the φ^4 model the collective coordinate approach can therefore not be used to establish that the shape mode is responsible for the existence of multiple bounces in kink–antikink scattering.

Though we have successfully waved a number of previous approximations within the ODE calculation, we have still omitted the interaction between the shape modes at $\pm X$. Otherwise the calculations run into the null–vector problem [18]. This problem arises because by pure construction of the ansatz, the coefficient of A vanishes for $X = 0$, *cf.* eq. (6). The particular combination of shape modes at $\pm X$ is commonly assumed because the more general parameterization with three collective coordinates (X, A, B)

$$\varphi_{\rm cc}(x,t) = \varphi_{K\overline{K}}(x, X(t)) + \sqrt{\tfrac{3}{2}}\left[A(t)\chi_1(x + X(t)) + B(t)\chi_1(x - X(t))\right] \qquad (20)$$

only yields a linear source term for $A-B$. Of course, the combination $A+B$ will nevertheless be excited by non–linear and/or higher order effects. It will therefore be interesting to investigate the above parameterization. This will complicate the collective coordinate approach slightly as it turns it into a 3×3 problem. Beyond that, the ODE approach is probably no longer a sensible simplification to the PDE.

Acknowledgments

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