Chapter 5

Applications

In this chapter we apply the perturbation methods developed in Chapters 3 and 4 to several representative examples of different classes of physically interesting perturbations. The first-order motion is always relatively easy to obtain as it only involves solving for the ψ_0 field (even this is not necessary for certain coupling functions $F[\Phi, \Phi_x]$) and then evaluating numerical integrals such as

$$\int_{-\infty}^{\infty} dx \; v(x+X)\phi_c(x) \; .$$

Once the effective potential is known the first-order motion of the kink center of mass variable X is qualitatively known. It is the second-order motion which requires a bit of numerical effort. In the following section the numerical procedure followed to calculate the second-order kink motion is outlined. The codes themselves are not included as appendices because they would require at least 100 pages of text (at least 60% of this is documentation). In section 5.2 we examine the procedure used to obtain the phonon field $\psi(x,t)$. Then in section 5.3 we treat the interaction of a kink with a time-independent, spatially localized perturbation. The effects of a uniform force on a sine-Gordon kink are studied in section 5.4. In section 5.5 the oscillatory motion of a kink in a binding symmetric well is considered. Finally, in section 5.6 we study the motion of a kink traveling in a medium whose limiting propagation speed changes smoothly to a higher value.

5.1 The Numerical Procedure

The set of equations which need to be solved to obtain the kink motion through second order is

$$(M_0 \quad + \quad \xi)\ddot{X} = -\frac{\partial V(X,t)}{\partial X} + \frac{1}{2}\int \chi^2(x,t)U'''[\phi_c(x)]\phi_c'(x) - 2\dot{X}\int \dot{\psi}'\phi_c'$$

$$
\begin{aligned}
&- \int v(x,t)\Big[\chi(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c} + \chi'(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c'}\Big] \\
&- \dot{X}^2 \int \dot{\psi}'\phi_c'(x) \ , \qquad (5.1.1)
\end{aligned}
$$

$$
\begin{aligned}
\ddot{\psi}(x,t) &- \psi''(x,t) + \psi(x,t)U''(\phi_c) = (1-\mathcal{P}_{\phi_c})\Big\{\Big[1-U''(\phi_c)\Big]\psi_0(x+X,t) \\
&+ v(x+X,t)\Big[F_{10}[\phi_c,\phi_c'] - F_{10}[0,0]\Big] \\
&- \frac{d}{dx}\Big[v(x+X,t)\Big(F_{01}[\phi_c,\phi_c'] - F_{01}[0,0]\Big)\Big]\Big\} \ , \qquad (5.1.2)
\end{aligned}
$$

where

$$\chi(x,t) = \psi(x,t) + \psi_0(x+X,t) \qquad (5.1.3)$$

$$V(X) = -\int_{-\infty}^{\infty} v(x+X)F[\phi_c(x),\phi_c'(x)] \ . \qquad (5.1.4)$$

The expression for the effective potential $V(X)$ differs from the more general expression given in Eq. (3.4.8) because the codes are currently set up to handle only perturbations $v(x)$ which are independent of time.

The first step is to compute the effective potential $V(X)$ for the range of X which is to be examined. Typically $V(X)$ will go to zero for $X < X_{bgn}$ and $X > X_{end}$ so the numerical integrals need only to be computed for a finite range of X. Up to 200 values of $V(X)$ are calculated for evenly spaced $X_{bgn} < X < X_{end}$. A bi-cubic spline fit [96] is then made to these data points, points outside the "nonzero" range being set to zero. To be certain that the spline routine is working properly, both the raw data points and interpolated values of $V(X)$ are plotted and compared. This check is made each time such spline coefficients are needed.

Given $V(X)$ the first order motion of the kink is calculated by numerically integrating the first order equation

$$\ddot{X} = -\frac{\partial V(X,t)}{\partial X} \ , \qquad (5.1.5)$$

by using the algebraic/differential system solver DASSL [97]. Once again a spline fit is made to the data points and the spline coefficients are written to a data file for later use.

The next step is to evaluate the background field ψ_0 which obeys the following equation

$$[\partial_{tt} - \partial_{xx}]\psi_0(x,t) + \psi_0 U'(\psi_0) - F_{10}[\psi_0,\psi_0']v(x,t) + \frac{d}{dx}(v(x,t)F_{01}[\psi_0,\psi_0']) = 0 \ . \qquad (5.1.6)$$

Since this is a linear equation it is possible to solve it by using fast Fourier transforms. In using the fast Fourier transform codes found in the standard subroutine libraries, one must be careful to include all of the appropriate scale factors. That this has been done properly was checked by comparing the numerical results with analytic results which are available for a special perturbation.

Now all of the functions needed to compute the right-hand side of the ψ PDE are contained in spline coefficients. Evaluation of this inhomogeneous term again involves some numerical integrals. Since this inhomogeneous term has $1-\mathcal{P}_{\phi_c}$ as a prefactor, it must be orthogonal to the translation mode $\phi_c'(x)$. This orthogonality relation is explicitly checked by evaluating the integral

$$\int_{-\infty}^{\infty} dx\ \phi_c'(x) I(x,t)\ , \tag{5.1.7}$$

with $I(x',t')$ given by the right-hand side of Eq. (5.1.2), for as many as 200 values of t. This is also a check on the spline fit since the values of the integrand are obtained from the spline functions.

Now we are in a position to solve the ψ PDE numerically. A numerical method which utilizes the method of lines [88] is used for this step in the calculation. The boundary conditions applied to solve the PDE are that ψ be zero at both ends. That this is the correct boundary condition may be seen by noting that any phonons which propagate to the boundaries take a finite amount of time to reach them so given any value of time t, one can find a value of $x = x_0$ such that $\psi(x,t) = 0$ for $x > |x_0|$. Of course one cannot make the simulated system arbitrarily large without using lots of computer time. Therefore one must be on the watch for effects of radiation which reflects off of the boundary. One of the checks made to both monitor this radiation problem and to check the PDE solver is to take the values of ψ obtained and substitute them back into the PDE. The PDE does not "know" about radiation which has been reflected from the walls so if the numerically calculated values of ψ and its derivatives satisify Eq. (5.1.2), we know the codes are working correctly (again, this also checks the spline fits). One of the additional rather nice features of the code is that one can take many snapshots of the ψ field and run them as a movie on a Sun computer. This method of viewing the phonon field can be more efficient than looking at the two-dimensional surface described by $\psi(x,t)$.

A rather subtle point remains to be discussed regards the numerical evaluation of the ψ field. When one views the plots of $\psi(x,t)$ vs. x and t, there appears to be a contribution which is not orthogonal to the translation mode. This fact is confirmed by numerical integration and therefore one searches for the source of the error. In fact one finds no error in the numerical method implemented, rather the cause of the trouble lies in the form of the ψ equation itself

$$\psi_{tt} - \psi_{xx} + U''[\phi_c(x)]\psi = I(x,t) \ . \tag{5.1.8}$$

The solution of this equation is required to be orthogonal to the translation mode $\phi'_c(x)$, however this PDE does not "know" about this constraint. In fact, this equation is linearly unstable to the translation mode. To clarify this statement, consider adding a time dependent constant times the translation mode to the actual solution desired, denoted by $\psi_\perp(x,t)$;

$$\psi(x,t) = \psi_\perp(x,t) + \alpha(t)\phi'_c(x) \ . \tag{5.1.9}$$

Since $\psi_\perp(x,t)$ is assumed to satisify Eq. (5.1.8), substitution of Eq. (5.1.9) into (5.1.8) yields the following equation for α:

$$\alpha_{tt}\phi'_c(x) - \alpha(t)\phi'''_c(x) + \alpha(t)\phi'_c(x)U''[\phi'_c(x)] = 0 \ , \tag{5.1.10}$$

which can be rewritten as

$$\alpha_{tt}\phi'_c(x) - \alpha(t)\phi'''_c(x) + \alpha(t)\frac{d}{dx}U'[\phi'_c(x)] = 0 \ . \tag{5.1.11}$$

Next, using the fact that $U'[\phi_c(x)] = \phi''_c(x)$, we see that the last two terms cancel leaving us with

$$\alpha_{tt}\phi'_c(x) = 0 \ . \tag{5.1.12}$$

Therefore we see that $\alpha(t)$ can grow linearly with t and we still have a solution of Eq. (5.1.8). Therefore, if in the numerical integration of the PDE, contributions proportional to $\phi'_c(x)$ will grow linearly. There are probably quite elaborate methods to prevent this which involve a modification of the PDE solver. Since this is a nontrivial procedure, we resort to allowing this linear growth to occur, projecting it out after the entire ψ field is obtained. As a final check, this resulting field is again substituted into the PDE, good agreement being attained.

The final steps required to obtain $X(t)$ to second order involve more numerical integrals of functions found on the right-hand side of Eq. (5.1.1) and then numerical integration of this ODE governing X.

Since there are several nontrivial numerical steps needed in this perturbation procedure, one must ask how accurate the final answer is. Although there are quite a few steps needed, each result obtained is either compared with analytic results when available or an indirect property, such as orthogonality to a given function is checked. Therefore we say with confidence that the final second-order result for $X(t)$ is accurate to at least two or three significant digits. This number could undoubtedly be pushed further since the tolerances presently being requested are not at their absolute limit. However this could entail the consumption of several hours of Cray-1 time with no better physical understanding. Of course such added significant digits would not be relevant since higher order corrections would wash out this accuracy. Currently the total time required to do all of the calculations for the second-order kink motion (including all relevant plots) is approximately two minutes of Cray-1 time. Therefore these calculations are quite tractable in at most a few hours of time on a personal computer.

5.2 Evaluation of $\psi(x,t)$

Since the ψ field satisfies a PDE it is the most difficult part of the numerical scheme. As mentioned above this problem has been solved by actually integrating the PDE. In this section we present some other methods which, although haven't proven to be as efficient as the PDE solver, are nonetheless legitimate methods.

The first method which comes to mind is the use of the Green functions derived in Chapter 4. This approach is the method of choice because one does not have to deal with such problems as reflected radiation from the boundaries. However, it does require the numerical evaluation of a two dimensional integral. There are several packaged routines which are set up to do such integrals. However, they work best when the integrand is a smooth function which is not the case as can be seen in Figure 5.1 for the perturbation discussed in section 5.3. The rapid oscillations in time are due to the Green function, so this method would be quite efficient if the perturbation was such that the function $I(x',t')$ did not sample so many oscillations. Even when it does sample many oscillations, the two dimensional numerical integrator works. However, to accurately do one such integral to an accuracy of three significant digits requires about one minute of Cray-1 time. Since the $\psi(x,t)$ field is needed for approximately 30 values of x and 100 values of t, this computation would require hours of Cray time.

The use of a Fourier transform method has been ruled out in Chapter 4 due to the step function in $G(x,x',t-t')$ at the "light cone". A Laplace transform method was then shown to circumvent this step function. However, since the question of the oscillations discussed in section 4.3 has not yet been resolved, this method has not been implemented. A method which would require the use of the Green functions evaluated at complex arguments requires a deformation of the contour from along the real time axis into the complex t plane (see Figure 5.2). The complex component of time would add an exponentially decreasing factor to the integrand which would greatly enhance convergence. This method has not been implemented because at present the modified Lommel function codes are not set up to handle complex arguments.

At this point it was decided to solve the ψ PDE itself. Since it is a linear equation, there are several techniques available. One can Fourier transform in

Figure 5.1: The integrand $G^{SG}(x, x', t - t')I(x', t')$ for $x = 50$, $t = 25$. The inhomogeneous function I corresponds to the perturbation studied in section 5.3.

Figure 5.2: Deformation into the complex t plane of the contour for the integral representation of $\psi(x,t)$ (see Eq. (3.4.12)).

time,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \bar{\psi}(x,\omega) \ , \tag{5.2.1}$$

which then requires the solution of the complex ODE

$$-\omega^2 \bar{\psi} - \bar{\psi}_{xx} + U''(\phi_c)\bar{\psi} = \bar{I}(x,\omega) \tag{5.2.2}$$

where $\bar{I}(x,\omega)$ is the Fourier transform of the inhomogeneous term $I(x,t)$. The solution of this ODE is certainly easier than solving a PDE. However one needs to invert the Fourier transform to obtain $\psi(x,t)$. This method of attack is not implemented because it requires far more CPU time than the PDE solver.

One final method involves doing a discrete time Fourier transform, that is using fast Fourier transform packages. This requires the solution of $2N+1$ coupled ODEs for the Fourier coefficients $c_n(x)$ and $s_n(x)$ defined by

$$\psi(x,t) = \sum_{n=0}^{N} c_n(x) \cos\Big[\frac{2n\pi(t - t_{bgn})}{t_{end} - t_{bgn}}\Big] + \sum_{n=0}^{N} s_n(x) \sin\Big[\frac{2n\pi(t - t_{bgn})}{t_{end} - t_{bgn}}\Big] \ . \tag{5.2.3}$$

Even by using the fastest fast Fourier transform codes available this procedure requires more time than the PDE solver. Although there are dangers in using the PDE solver (e.g., reflected radiation), it has the advantage that it requires only one step, namely the solution of the PDE. The Fourier transform methods outlined require the evaluation of Fourier transforms, solution of ODEs and then the inverse transforms. Each additional step adds to the unavoidable round-off errors.

5.3 Kink Collision with a Localized Impurity

For our first application of the method outlined above we consider the motion of a sine-Gordon kink in the presence of a a time-independent perturbation $v(x)$ which is localized in space. The coupling function $F[\Phi, \Phi_x]$ is chosen to be $\Phi(x,t)$ so that the interaction Hamiltonian has the form

$$H_{int} = -\int_{-\infty}^{\infty} dx \ v(x) \ \Phi(x,t) \ . \tag{5.3.1}$$

The choice of the perturbation $v(x)$ is motivated by an example studied by FTBK [37] who chose for their interaction Hamiltonian

$$H_{int} = -\int_{-\infty}^{\infty} dx \ u(x) \ \Phi'(x,t) \ . \tag{5.3.2}$$

Figure 5.3: The perturbation $v(x)$ (solid) and the background response $\psi_0(x)$ (dashed) it generates.

where $u(x)$ is the sum of two step functions. In the language of charge-density-wave systems, the derivative of the field Φ_x represents the local, excess charge density. Therefore, the perturbation given in Eq. (5.3.2) models the interaction of a charge-density-wave with two defects of opposite strength. By integrating Eq. (5.3.2) by parts we obtain a form analogous to Eq. (5.3.1) with $v(x)$ the sum of two delta functions. To make the perturbation more realistic, we replace the two delta functions by Gaussians of width w^{-1} and centered at $\pm x_0$

$$v(x) = \lambda \Big\{ e^{-w(x-x_0)^2} - e^{-w(x+x_0)^2} \Big\} \ . \qquad (5.3.3)$$

Using Eq. (5.1.6) with $F_{10} = 1$ and $F_{01} = 0$, we numerically determine the background response $\psi_0(x,t)$ induced by $v(x)$. Due to the simple form of $v(x)$ an analytic expression for the ψ_0 field is available in terms of the complementary error function. This expression agrees very well with the numerical computation of ψ_0 which is plotted in Figure 5.3 along with the perturbation for the following parameter values

$$X(0) = -20 \quad , \quad \dot{X}(0) = 0.3 \quad , \quad \lambda = 0.04 \quad , \quad w = 1 \quad , \quad x_0 = 5 \ . \qquad (5.3.4)$$

As one would expect, a localized perturbation leads to a localized response. The effective potential which the kink feels in first order is given by

$$V(X) = - \int_{-\infty}^{\infty} dx \ v(x+X) \phi_c'(x) \ , \qquad (5.3.5)$$

Figure 5.4: The potential $V(X)$ (solid) and its derivative $V'(X)$ (dashed).

and is plotted in Figure 5.4 with the negative of the effective force $V'(X)$. From this potential energy graph, we see that the velocity of the kink center of mass should increase upon entering the perturbation region and then decrease upon leaving. This behavior is confirmed when the first-order equation of motion is solved numerically, the results of which are plotted in Figure 5.5. These first-order results are quite reasonable when one physically examines the perturbation chosen in the context of the sine-Gordon pendulum chain. In this case, the perturbation given by Eq. (5.3.1) may be interpreted as representing two equal but opposite localized torques acting on the chain. The first of these torques pushes the pendula to positive angles and therefore tends to aid in the propagation of the kink whereas the second has the opposite affect. Therefore a simple physical argument gives us our first-order results. Such arguments are not available when we want to consider the second-order motion which represents the effects of the phonons back on the kink center of mass.

Before we can study the second-order motion of the kink center of mass, we must solve for the radiation field $\psi(x,t)$. For this type of perturbation, we found that the easiest way to solve for ψ is by direct numerical integration of the PDE given in Eq. (5.1.2). The first step in this process is the evaluation of the inhomogeneous term in the ψ PDE which for the present perturbation is

$$(1-\mathcal{P}_{\phi_c})\Big[1-U''(\phi_c)\Big]\psi_0(x+X,t)\ . \tag{5.3.6}$$

Although an analytic form for ψ_0 is available, we were unable to get an analytic result for the integral in Eq. (5.3.6) [the integration is implied by the projection

Figure 5.5: The first-order kink position $X(t)$ (solid) and velocity $\dot{X}(t)$ (dashed).

operator $\mathcal{P}_{\phi_c}$] and therefore had to resort to a numerical evaluation. The result of this calculation must be orthogonal to the translation mode, a fact which was confirmed by explicit numerical integration over x for 100 evenly spaced values of time. Finally we note that we used the first-order result for $X(t)$ in evaluating Eq. (5.3.6).

The numerical technique used to solve the PDE is a method of lines technique developed by J. M. Hyman [88]. Although this code has proved to be quite reliable in a variety of problems, we made the further check of substituting the values obtained for ψ back into the PDE and obtained good agreement. The results of the numerical integrations are given in Figure 5.6. Initially the ψ field is zero and attains nonzero values only the kink encounters the first of the Gaussian perturbations. After the kink has passed the second Gaussian perturbation, the ψ field appears to go to zero. The dominant features shown in Figure 5.6 represent a temporary shape change of the kink. In addition we see that some small amplitude radiation is emitted in the collision process. One can see this radiation propagating towards the boundary which eventually reflects back toward the center of the system. The length of the system was chosen so that for the times examined this reflected radiation does not influence the motion of the kink.

Given the ψ and ψ_0 fields, we perform the appropriate integrals over space as required in Eq. (5.1.1) which enables us to solve the second-order equation of motion for X. Since the second-order corrections to the velocity are quite small, we plot only this contribution, labeled by δv, in Figure 5.7. Figure 5.7 shows that the second-order contribution to the kink velocity experiences an increase followed by

Figure 5.6: Phonon field $\psi(x,t)$ generated during the collision of the kink with the impurity.

Figure 5.7: The second-order contribution to the kink velocity.

a sharp decrease, which corresponds to the collision with the first of the Gaussian perturbations. Next the velocity moves towards zero before undergoing a decrease followed by an increase before settling into oscillations, that is upon encountering the second Gaussian perturbation the velocity changes in essentially the same fashion as it did as when it "hit" the first, but in reverse order.

The small oscillations which are present after the collision have a mean which is slightly smaller than the initial velocity. This slightly reduced velocity represents a transfer of energy into the radiation field. The oscillations in the velocity demonstrate the fact that the kink is indeed a deformable particle. Similar oscillations in the kink velocity have been observed in kink-antikink scattering in ϕ^4 [15]. Campbell et al. [15] have demonstrated explicitly that this type of "wobbling kink" is the result of an exchange of energy between the kink and the "shape mode". (See §6.1 for a detailed discussion of this energy exchange). In addition, Segur has presented analytic evidence for the existence of "wobbling kink" solutions in ϕ^4 [43]. The ϕ^4 wobbling kinks were found to be stable while the sine-Gordon kinks were found to be mildly unstable [43].

Although we cannot follow the evolution of the velocity for arbitrarily large times, we know from the analysis given in section 3.4 that the kink will eventually reach a constant velocity because our perturbation is localized and time-independent. Although the value of the final velocity is only slightly less than the initial velocity, the difference in the kink position due to this second order effect relative to first-order result will grow linearly in time which would hopefully be a measurable quantity. Since the ψ field depends linearly on the perturbation strength λ, we should see a quadratic growth with λ in this second-order effect. A more systematic study of this perturbation is planned to examine the dependence of this effect on the parameters λ, w, and x_0. It would also be interesting to treat the repulsive potential ($\lambda < 0$) to study the reflection of kinks. It is conceivable that with the additional freedom gained by allowing the kink shape to deform, (i.e. the ψ field effectively changes the shape of the kink) one could see transmission of a kink in second order when reflection occurred in first order ("classical tunneling") [98].

5.4 Uniform Force with Damping

Next we study the motion of a kink under the influence of a uniform force that is, a perturbation which is independent of space and time. In addition we add a phenomenological damping term to simulate the effect of fluctuations experienced in real systems. The source of this dissipation varies from the ordinary lattice vibrations [64] present in solids to shunt resistances in Josephson junctions [17] to interchain coupling in polyacetylene [19].

This particular perturbation has been the source of a great deal of controversy. In a series of papers Fernandez, Reinisch, and coworkers [85] claimed to observe non-Newtonian motion of the kinks. Specifically they found that for small times the kink position grew as t^3 compared with the standard result of t^2 for a particle under the influence of a constant force. For longer times the t^2 behavior was observed. Since then several investigators [99, 100, 101] have pointed out that in their work, Fernandez et al. did not account for the background response of the field explicitly. Specifically, their initial condition was a sine-Gordon kink without including the uniform background shift produced by a constant force. Therefore their evolution equations had to generate this background in addition to accelerating the kink. After a short time this constant background was established and from then on Newtonian acceleration of the kink was observed.

Although the formalism developed so far can be used to treat such a perturbation, we will make use of results derived in Appendix B. There we show that we can derive the kink center of mass equation by simply substituting the field ansatz of Eq. (2.3.2) into the equation of motion for the full $\Phi(x,t)$ field. This simple substitution is possible because the transformation equations give us the old variables in terms of the new ones. In addition to giving the correct equations of motion with less effort, this procedure allows us to add a phenomenological damping term. We take as our coupling function $F[\Phi, \Phi_x] = \Phi$ and $v(x,t) = E_0$ as the perturbation which gives us

$$\Phi_{tt} + \epsilon\Phi_t(x,t) - \Phi_{xx} + U'(\Phi) - E_0 = 0 \ . \tag{5.4.1}$$

Substitution of Eq. (3.3.2) into Eq. (5.4.1) yields the following first-order equation of motion for the kink center of mass

$$M_0\ddot{X} = 2\pi E_0 - \epsilon\dot{X} \ , \tag{5.4.2}$$

where we have assumed that the damping parameter ϵ and constant force E_0 are both small and of the same order. Equation (5.4.2) states that for $\epsilon = 0$ the kink undergoes constant acceleration for all times. We see no evidence of non-Newtonian behavior because our method explicitly accounts for the motion of the "wings", that is the regions far from the kink center (as suggested by Olsen and Samuelson [100]). In this case, the ψ_0 field ("wings") is simply given by

$$U'(\psi_0) = E_0 \ . \tag{5.4.3}$$

To obtain the full field $\Phi(x,t)$, one would have to add in the background contribution ψ_0 plus any phonons produced.

Another way to study a space- and time-independent perturbation is to include the constant background ψ_0 in the definition of the kink [101, 102], that is we define a "deformed kink" $\phi_c^D(x)$ which satisifies

$$-\partial_{xx}\phi_c^D + U'(\phi_c^D) + E_0 = 0 \ . \tag{5.4.4}$$

Both methods (Euler-Lagrange and "direct substitution") for deriving the equation of motion for the kink center of mass variable are still valid when one uses the deformed kink because the only feature that one exploits is that the kink satisfies a given differential equation. However, when the full field $\Phi(x,t)$ is decomposed into a deformed kink plus a radiation field, the question of the stability of this ansatz against small oscillations must again be addressed. Therefore we proceed as before, assuming that the field can be decomposed into a "deformed kink" plus a phonon field $\psi(x,t)$,

$$\Phi(x,t) = \phi_c^D(x) + \psi(x,t) \ , \tag{5.4.5}$$

where the deformed kink $\phi_c^D(x)$ satisifies Eq. (5.4.4). Using Eq. (5.4.3), one can show that $\psi(x,t)$ satisifies

$$\psi_{tt} - \psi_{xx} + \psi U''[\phi_c^D(x)] = 0 \ . \tag{5.4.6}$$

Equation (5.4.6) differs from Eq. (3.1.6) only in that the second derivative of the potential is evaluated at the deformed kink. Since the perturbation is assumed small, the change in the spectrum of the operator in Eq. (5.4.6) is small. In particular, there is still a zero frequency mode present. If our ansatz is unstable, there must be a mode whose squared frequency is negative. Since we still have a zero frequency mode, this means that the eigenvalue of one of the bound state modes or continuum modes must be less than zero. Since our perturbation is small, first order perturbation theory tells us that the change in the eigenvalues of these modes must also be small and therefore no such negative eigenvalue is possible for small perturbations. The result of this analysis is that the deformed kink also obeys Newton's law as stated in Eq. (5.1.1) in which the background field $\psi_0(x) = 0$. Although this result can be obtained without referring to a deformed kink, the fact that one can use a deformed kink as a starting point turns out to be very useful when the problem of thermal noise is attacked via a Fokker-Planck approach (see section 6.3.6).

5.5 Oscillation in a Binding Symmetric Potential

In this section we investigate the motion of a sine-Gordon kink under a time-independent perturbation $v(x)$ which for small x has a quadratic minimum at $x = 0$. The trapping or pinning of solitons is a phenomenon which has attracted quite a bit of attention lately [103, 104, 105]. Once again the theme is the exchange of energy from the solitons into other modes of the system. In what follows we present a rather general analysis, which although it is of limited applicability due to the approximations made, shows some techniques which may be applied to obtain detailed second order results without resorting to numerical analysis. Following this we present some preliminary numerical results.

We choose as our coupling function $F[\Phi, \Phi_x] = \Phi_x$ which as shown below will lead to a symmetric binding effective potential for the kink. To see that this is indeed the case, we make a Taylor series expansion of the effective potential

$$V(X) = \lambda \int_{-\infty}^{\infty} dx\ v(x+X)\phi_c'(x)\ . \tag{5.5.1}$$

about $X = 0$. Such an expansion is valid for low energy kinks, that is for both $X(0)$ and $\dot{X}(0) \approx 0$. Carrying out this expansion we have

$$\begin{aligned} V(X) &\approx \frac{\lambda}{2}X^2 \int_{-\infty}^{\infty} v''(x)\phi_c'(x) + O(X^4)\ , & (5.5.2) \\ &\approx \frac{1}{2}\kappa X^2 + O(X^4)\ , & (5.5.3) \end{aligned}$$

where we have neglected a constant term and used the symmetry of $v(x)$ and $\phi_c'(x)$. Since $v''(x)$ and $\phi_c'(x)$ are both positive even functions, we see that the effective spring constant κ

$$\kappa \equiv \lambda \int_{-\infty}^{\infty} dx\ v''(x)\phi_c'(x)\ , \tag{5.5.4}$$

is positive.

We now consider the second-order motion of the kink, obtaining some general results without resorting to detailed numerical calculations. The second-order equation of motion, again assuming that the $\dot{X}^2$ term is negligible, may be obtained from Eq. (5.1.1)

$$(M_0+\xi)\ddot{X} = -\frac{\partial V(X,t)}{\partial X} + \frac{1}{2}\int \chi^2(x,t)U'''[\phi_c(x)]\phi_c'(x) - 2\dot{X}\int \dot{\psi}'\phi_c' \ . \qquad (5.5.5)$$

To examine the second-order terms in Eq. (5.5.5), we need some symmetry properties of the $\psi_0(x)$ and $\psi(x,t)$ fields. From Eq. (5.1.6) we have for the $\psi_0(x)$ field,

$$-\partial_{xx}\psi_0(x) + \psi_0(x) = v'(x) \ , \qquad (5.5.6)$$

where the appropriate Taylor series expansions have been used. Since $v'(x)$ is an odd function, $\psi_0(x)$ is also an odd function. In fact, for small x, $\psi_0(x) = x$ is a solution of Eq. (5.5.6) since $v'(x) = x$ for small x.

The ψ equation is given by

$$\ddot{\psi}(x,t) - \psi_{xx}(x,t) + \psi(x,t)U''[\phi_c(x)] = (1-\mathcal{P}_{\phi_c})\Big[1-U''(\phi_c)\Big]\psi_0(x) \ , \qquad (5.5.7)$$

where to lowest order we have replaced $X(t)$ by 0. This is the approximation which was mentioned above as seriously limiting the applicability of the following results. Since we can always obtain the first order center of mass motion before the ψ field is calculated, this approximation need not be made, however it allows us to continue with the analytic development.

To evaluate the ψ field we use the Green function representation,

$$\psi(x,t) = \int\limits_{-\infty}^{\infty} dx' \int\limits_{-\infty}^{\infty} dt' \Big[1-U''(\phi_c(x'))\Big]\psi_0(x') \int\limits_{-\infty}^{\infty} dk f_k^*(x) f_k(x') \int\limits_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_k^2-\omega^2)} \ , \qquad (5.5.8)$$

where we have also substituted the integral representation for the Green function ($\tau = t - t'$) and used the fact that $\phi_c'(x)$ is orthogonal to the functions $f_k(x)$. Since the only time dependence on the right-hand side of Eq. (5.5.8) occurs through the quantity $t - t'$, we can change the integration variable from t' to τ. After doing the τ and ω integrals we are left with

$$\psi(x) = \int\limits_{-\infty}^{\infty} dk \frac{f_k^*(x)}{\omega_k^2} \int\limits_{-\infty}^{\infty} dx' f_k(x') \Big[1-U''(\phi_c(x'))\Big]\psi_0(x') \ . \qquad (5.5.9)$$

Therefore to this order the ψ field is independent of time and hence the only remaining nonzero term in Eq. (5.5.5) which depends on ψ is ξ. Recalling the definition of ξ from Eq. (3.3.5) we have

$$\xi = \int_{-\infty}^{\infty} dx \psi'(x,t)\phi_c'(x) \; , \tag{5.5.10}$$

$$= \int_{-\infty}^{\infty} dx \phi_c'(x) \int_{-\infty}^{\infty} dk \frac{f_k^{*'}(x)}{\omega_k^2} \int_{-\infty}^{\infty} dx' f_k(x') \Big[1 - U''(\phi_c(x'))\Big] \psi_0(x') \; , \tag{5.5.11}$$

$$= - \int_{-\infty}^{\infty} dx' \Big[1 - U''(\phi_c(x'))\Big] \psi_0(x') \int_{-\infty}^{\infty} dk \frac{f_k^*(x')}{\omega_k^2} \int_{-\infty}^{\infty} dx f_k(x) \phi_c''(x) \; , \tag{5.5.12}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} dx' \Big[1 - U''(\phi_c(x'))\Big] \psi_0(x') x' \phi_c'(x') \; , \tag{5.5.13}$$

where we have made use of the identity in Eq. (3.1.15). Since $1 - U''(\phi_c(x')) = 2\text{sech}^2(x')$ and $\phi_c'(x) = 2\text{sech}(x')$ (both for sine-Gordon), and $\psi_0(x)$ is odd, we see that the mass renormalization is positive.

Now we consider a concrete example in which the perturbation has the form

$$v(x) = \lambda \; \text{sech} wx \; , \tag{5.5.14}$$

where the parameter values were chosen to be

$$w = 4 \quad , \quad \lambda = .04 \; . \tag{5.5.15}$$

In order to obtain oscillations (as opposed to escape to ∞) the initial conditions of the kink were taken as

$$X(0) = 0.0 \quad , \quad \dot{X}(0) = 0.05 \; . \tag{5.5.16}$$

In Figures 5.8 to 5.10 we present the perturbation, background, effective potential, and force along with the first order motion. As expected, the kink undergoes "harmonic-like" oscillations. Since in this example, the kink passes through the perturbation periodically, we might expect to see quite a few phonons generated, which is indeed the case as shown in Figure 5.11 Another interesting feature of the ψ field is that one can see that near $x = 0$ a slightly larger, more regular structure emerges, indicative of a permanent (or possibly periodic) shape change of the kink. One should also notice that the phonons emitted for small times reach the boundary quickly, and therefore almost certainly reflect back into the region of the perturbation, affecting the results. This is why these results were termed preliminary. Since the size of the system is already reasonably large, some other device such as absorbing boundary conditions will have to be employed in order to continue this study. One would also like to see more periods of the oscillation. However this involves increasing the effective spring constant κ which in turn means increasing the perturbation strength.

Figure 5.8: Perturbation (solid) and background field (dashed).

Figure 5.9: Effective potential (solid) and the negative of the force (dashed).

Figure 5.10: First-order kink position (solid) and velocity (dashed).

5.6 Transmission Through an Interface

As a final example we consider the effects of a change in the limiting speed of propagation of the kink. Such a change is commonly encountered in many physical systems in which some feature of the underlying medium undergoes a change. In Josephson junctions this situation arises when two such junctions with slightly different shunt capacitances are spliced together [17]. A change in the Fermi velocity, i.e. electron density, has a similar effect in charge-density-wave systems [106]. To model such changes we consider a perturbation of the form

$$H_{int} = \frac{\lambda}{2} \int_{-\infty}^{\infty} dx \; [1 + \tanh(x)] \Phi_x^2(x) \; , \tag{5.6.1}$$

which leads to the following modification of the equation of motion:

$$\Phi_{tt} - [1 + \lambda(1 + \tanh(x))]\Phi_{xx} - \lambda \mathrm{sech}^2(\mathrm{x})\Phi_\mathrm{x} + \sin\Phi = 0 \; , \tag{5.6.2}$$

where once again we consider the sine-Gordon system. Comparing Eq. (5.6.2) with Eq. (2.1.2), we see that we have a system in which the spring constant changes smoothly as a function of position. The term proportional to Φ_x results from the fact that the force on a given pendulum due to its left neighbor does not equal the force due to the right neighbor due to the variation in the spring constant.

The perturbation $v(x)$ and the negative of the effective force on the kink in first order are plotted in Figure 5.12. The background field ψ_0 in this case is

Figure 5.11: Phonon field $\psi(x,t)$. The length of the system is actually 60. However only a portion is shown here for clarity.

Figure 5.12: The potential (solid) and the negative of the effective force (dashed) for the interface perturbation.

Figure 5.13: The first order kink position (solid) and velocity (dashed) as a funciton of time.

zero which can be understood in terms of the sine-Gordon pendulum chain. From the equation of motion we see that the perturbation respresents a change in the limiting speed of the kink. This speed is in turn determined by the torsion spring constant. Therefore the perturbation in fact represents a change in the spring constant. Unlike the "torqued pendulum" perturbation studied in section 5.3, such a change in the spring constant does not give rise to any new equilibrium configuration of the pendula.

The resulting first-order motion of the kink is plotted in Figure 5.13. As mentioned in section 2.1, the "rest energy" of this system is proportional to the product of the limiting speed of the medium c_0 and the natural frequency ω_0. In our units $\omega_0 = 1$ so the rest energy is proportional to the limiting speed c_0. From Eq. (5.6.2) we see that this limiting speed depends on position and is given by

$$c_0^2(x) = 1 + \lambda(1 + \tanh(x)) \ . \tag{5.6.3}$$

Of course the interpretation of $c_0(x)$ as a limiting speed applies only when the term linear in Φ_x is zero, that is for large x. As $x \to \infty$ we find that the square of the limiting speed approaches $1 + 2\lambda$, and therefore for positive λ it increases.

This means that the "rest energy" also increases, so if the total energy is to be conserved, the velocity of the kink must decrease upon entering the perturbation region, as shown in Figure 5.13.

As in the previous examples, the interesting results occur in second order. In this case, we can physically deduce part of this contribution. Returning to space and time variables used in section 2.1, we recall that the width of a kink has the form

$$d = \frac{c_0}{\omega_0} \ , \tag{5.6.4}$$

where c_0^2 is the coefficient of the ϕ_{xx} term in Eq. (5.6.2) and ω_0^2 is the coefficient of the $\sin \Phi$ term. Since in Eq. (5.6.2) $\omega_0 = 1$, we see that the kink width is given by c_0. Therefore the width of the kink long after passing the interface must be

$$d = c_0 = \sqrt{1 + 2\lambda} \approx 1 + \lambda \ . \tag{5.6.5}$$

Any such shape changes in the kink must be taken up by the ψ field. In all of the previous examples this shape change has been localized in time. However in this case it must persist. Such qualitative behavior is shown in Figure 5.14, a change occurs when the kink encounters the interface and a constant profile is maintained thereafter with very few phonons emitted. To obtain a quantitative check, we plot (solid curve) in Figure 5.15 the difference between the final kink profile and the initial kink profile

$$\psi_{ana} = 4 \ \arctan(e^{x/(1+\lambda)}) - 4 \ \arctan(e^{x}) \ , \tag{5.6.6}$$

where the subscript ana denotes "analytic". On the same graph we plot the numerically evaluated ψ field (dashed) as a function of x for a given value of time for which the kink has passed the interface ($t = 80$). The agreement is quite remarkable, indicating the accuracy of the perturbation theory itself and the numerical method used in the calculation of the ψ field.

This ends the applications we have considered to date. They have been included as a means for demonstrating some of the features of the perturbation method developed in Chapter 3. One of the expected features is the exchange of energy from the kink center of mass motion into the phonon degrees of freedom, again indicating the deformable nature of the particle. On the other hand, the transmission through an interface illustrates the other role which the ψ field has, namely that of effecting a change of the kink profile. The agreement of the analytic and numerical plots for this deformation is quite impressive, giving us confidence not only with the perturbation theory, but with the numerical procedure employed. It remains to carry out some systematic studies of these and other perturbations to see, for example, how the number of phonons generated depends on the strength, width and shape of the perturbations and compare these results with the pertinent physical systems.

Figure 5.14: The phonon field $\psi(x,t)$ as a function of x and t for the interface problem.

Figure 5.15: Predicted (solid) and numerical (dashed) ψ fields.

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[153] See Ref. 89 p. 470, formula # 3.869.1.

[154] This result is incorrectly stated in Ref 91. Below Eq. (2) in §16.57, an error of 1/2 occurs; it should read:

$$\frac{1}{\pi}\int_0^\infty \frac{dt}{t}\sin[at+\frac{b}{t}] = J_0(2\sqrt{ab})$$

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[173] See Ref. 89 p. 967, formulae # 8.471.

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