Chapter 1

Introduction

In the past 20 years the study of nonlinear systems has experienced a large amount of attention [1]. Scientists in many branches have been coming to grips with the fact that the time-honored method of linearizing any nonlinearities that occur in their equations omits phenomena which are of great importance. At least two areas of research have emerged which account for these nonlinearities from the beginning. One of these areas has been termed Dynamical Systems [2, 3] which is the study of discrete maps and/or low dimensional sets of ordinary differential equations (ODEs). So far this branch of research has led to many interesting studies of turbulence, chaos, fractals, etc. Another branch which has received a great deal of attention is that of Nonlinear Waves [4, 5]. Here, the existence of special *solitary wave* solutions, that is, localized solutions which depend on x and t only through the argument $x - vt$, has indeed had a great impact on the scientific community. Of particular interest is a special type of solitary wave called a soliton which has the additional property that its shape and velocity are preserved asymptotically upon collisions with other solitary waves [6]. This is a familiar situation when one is dealing with a linear dispersionless system such as the wave equation in a dispersionless medium, however the addition of dispersion or nonlinearity tends to cause the shape of a pulse to spread or sharpen, respectively. It is therefore somewhat remarkable that when both dispersion and nonlinearities are present "in the correct proportions" that the spreading and sharpening exactly cancel, giving rise to solitons.

The first published observation of a solitary wave was made in 1834 by John Scott-Russell in his now famous report [7] of his chase of a "Wave of Translation" along a shallow canal. Since then, these waves have been produced in the laboratory and their properties investigated. In addition, the mathematical models which have solitary waves as solutions received much attention. The first evidence that such models could have soliton solutions was given by Perring and Skyrme [8] in 1962 in their numerical investigation of the sine-Gordon (SG) equation which indicated that after colliding, two of these solitary waves emerged with the same shape and velocity that they had long before they interacted. In 1965, Zabusky and Kruskal published results of a similar numerical investigation [9], this time using the Korteweg-deVries (KdV) model. These simulations led to analytic multi-*soliton* solutions which described the collisions. Soon an entire hierarchy of solitons was produced with the help of Bäcklund transformations [10] which create an "n-humped" solution to an "$n+1$-humped" solution. Further work involving a technique called the Inverse Scattering Transform [11] showed that for the infinite line, one could actually find action-angle variables for the sine-Gordon and KdV models. Soon other integrable models including the nonlinear Schrödinger equation [12], Boussinesq [13] , modified KdV [14], etc. were discovered, adding to the set of evolution equations which yield solitons. In addition to the growing list of integrable systems which support N-soliton solutions, nonintegrable models were also found in which solitary waves exist and have nearly elastic collisions [15]. One of the most well known nonintegrable models is the ϕ^4 theory. In this case, one does have an analytic form for a solitary wave, however one cannot use the beautiful machinery of Bäcklund transformations or the Inverse Scattering Transform methods to generate and/or study soliton solutions. Although this removes one of the only nonperturbative tools for investigating solitary waves, it has not stopped efforts as is evidenced by the large number of applications found for nonintegrable as well as integrable models.

It is of course the applications of these models which are of interest to the physicist. Scott-Russell's observation of a solitary wave in water was the first study of a soliton-bearing physical system. Since then, solitary waves have found their way into more modern applications such as Langmuir waves in plasmas [16], Josephson junctions [17], quasi-one-dimensional magnets [18], charge-density-waves [19] and dislocations [20] to name a few. Not only are solitons present in these samples, but they can also contribute strongly to such processes as conduction, photoabsorption, magnetization, etc. In fact there are examples in which the normal mechanisms which lead to the above physical processes are for some reason inhibited and the conduction for example is mainly due to the motion of solitons.

There is perhaps there is no better illustration of this than the Josephson junction in which quanta of flux called "fluxons" are observed to propagate along the insulating barrier separating the two superconducting strips [21, 22, 23, 24, 25, 26]. The standard model which approximately describes the phase difference across a Josephson junction is the sine-Gordon equation [27]. To more closely mimic the actual physical situation, additional terms representing driving bias current and dissipation are added to the sine-Gordon equation. Since the resulting equations are not exactly solvable, one must develop perturbation schemes to obtain approximate solutions. Several such schemes have been proposed in recent years, not only for the sine-Gordon equation, but for many of the nonlinear wave equations mentioned above.

Many of these perturbation theories are based on the fact that although one cannot obtain an exact solution merely by a specification of the motion of the solitary waves, such a description can often provide a good first approximation. This situation is familiar in the study of nonlinear systems and is not confined to solitary wave bearing systems. Consider, for example, the flow of a viscous fluid in which vortices are present. To the extent that the Navier-Stokes equation describes this system, one can obtain an "exact" solution by solving it. However, this involves the solution of a three-dimensional partial differential equation (infinite-dimensional system of ODEs). An approximate solution can often be obtained if one concentrates on the motion of the vortices themselves. In this way one can achieve a drastic reduction in the dimensionality of the system of ODEs. Instead of solving the Navier-Stokes equation, one can obtain an approximate solution by studying the motion of a few extended particles (vortices) whose interactions can be characterized by an attractive or repulsive potential. A similar situation occurs in the study of shock wave propagation in which one identifies a shock front and focuses attention on the front itself instead of the entire flow field.

This type of analysis has proved fruitful in nonlinear systems which support solitary wave solutions. The systems to which we shall confine our attention to are those which have "kink solitary wave" solutions, that is a system in which one or more of the quantities, such as the spin orientation in a ferromagnetic domain wall, undergoes a smooth change from one value to another. In both experments and numerical simulations it has been observed that the motion of these kinks dominates to the point that in a first approximation, the entire system is describable by merely prescribing the positions and velocities of these modes as a function of time. It is therefore quite natural to attempt to describe such systems by assigning a position coordinate to the solitary wave and derive equations which describe the evolution of such "collective coordinates" and/or interactions between these coordinates. For the systems studied in this work, this approach is particularly rewarding as we find that the collective coordinate which describes the motion of a kink obeys Newtonian dynamics. That is not to say that these kinks behave as point Newtonian particles. Rather, the extended nature of these normal modes gives these "particles" extra "degrees of freedom" such as shape oscillation.

Recall that the motion of these normal modes describes the system only to a first approximation. Often one finds that the deviation between this first approximation and the actual behavior consists of small fluctuations about the nonlinear modes. Such fluctuations, termed "phonons", must also be accounted for if a more complete description of the system is to be obtained. Not only must the generation of such phonons be described, but in addition one must also account for any effect that the phonons may have back on the motion of the kinks themselves. The perturbation theory developed in Chapter 3 takes all such considerations into account. The kink position is regarded as a collective coordinate and is found to obey a Newtonian equation of motion. To a first approximation, one can describe the entire system by an effective potential in which the kink moves. To obtain corrections to this motion one must first compute the phonon field generated, a task accomplished by solving a partial differential equation satisified by the phonon field. This field in turn enters into the second-order equation of motion for the kink position, indicating that the emitted phonons do indeed have an effect on the motion of the kink.

In addition to influencing the motion of the kink and describing the emission of phonons, the phonon field can also account for a temporary or permanent shape change of the kink. In the examples presented in Chapter 5, both features of the phonon field are illustrated. In one example we find that the kink experiences a temporary shape change as it passes through a localized perturbing influence. In addition to this temporary change, the interaction produces some phonons. The effect of these phonons on the kink motion is to cause the velocity of the kink to oscillate with small amplitude about the final velocity which is slightly below the initial velocity. This process again illustrates the fact that the kink is an extended, deformable particle. The phonon degrees of freedom allow for a transfer of energy between the kink translational motion and the other degrees of freedom. This interaction is one of the most interesting aspects of the present perturbation theory.

One of the perturbations for which the theory of Chapter 3 is not well-suited concerns the addition of a fluctuating force plus a phenomenological damping term as occurs in kink-bearing systems at finite temperature. Motivated by studies of a single particle under the influence of a fluctuating forces and damping, we apply both Langevin and Fokker-Planck methods to analyze the stochastic kink dynamics in Chapter 6. The results of these calculations echo the results of the deterministic perturbation theory of Chapter 3, namely to lowest order the kink behaves as an ordinary (Brownian) particle. The effect of the phonons is to add temperature dependent corrections to the mass and diffusion constant. Much of the analysis in Chapter 6 describes formal work which is needed to complete the detailed calculations which are required for the higher order corrections.

All of the work mentioned above is based on a canonical transformation to a set of “kink variables” which represent the kink position and the momentum conjugate to the kink position. The existence of such a transformation places the entire perturbation theory on a very firm foundation. However, one cannot always expect to find such a canonical transformation. Indeed, one would hope that such a transformation is not necessary in order to obtain an accurate description of the system. Rather, one would like to identify the relevant collective coordinates from the actual physical phenomena or numerical simulations. More precisely, one would like to be able to make a simple ansatz for the various fields (such as the spin) which is based on these collective coordinates. Such a collective-coordinate ansatz is applied to kink-antikink collisions in phi-4 field theory in Chapter 7. Results indicate that the most obvious use of the collective coordinates does not capture the behavior found in the simulations of the PDE. An alternate ansatz which includes "relativistic" effects is proposed and briefly discussed.

Chapter 2

Background and Previous Work

In this chapter we shall briefly review several of the perturbation theories which are already in use. Many of these methods are based on the use of collective coordinates, although in some cases this is more evident. Since many of these methods are mathematically rather involved, it is useful to become aquainted with a familiar model nonlinear system which one can refer to in order to use one's physical insight to help understand the perturbation methods and the results obtained from these methods. To this end we begin this chapter with a discussion of the sine-Gordon pendulum chain.

2.1 The sine-Gordon Pendulum Chain

Although any of the physical systems mentioned in Chapter 1 could serve as a model to exhibit some of the properties of solitons, it is perhaps easier to use a mechanical model, the sine-Gordon pendulum chain. This model has long served as a paradigm [23] which exhibits many of the generic properties of systems bearing solitons. It's use has not been limited to gaining a rudimentary knowledge of a typical integrable nonlinear system, but also to understand some of the more advanced concepts such as homoclinic orbits, separatrices etc. which one encounters when one studies the transition to chaos [28].

The sine-Gordon pendulum chain consists of a chain of pendula separated by a distance a and connected to one another by (linear) springs with torsion constant κ as shown in Figure 2.1. The entire chain is in a gravitational field and therefore the equations of motion which describe the angular deviation Φ_n of each pendulum from vertical are given by

$$I\frac{\partial^2\Phi_n}{\partial t^2} = \kappa[\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}] - mgl\sin\Phi \ , \tag{2.1.1}$$

where $I = ml^2$ is the moment of inertia of one of the pendula, m is the mass, l

Figure 2.1: The sine-Gordon pendulum chain.

is the length and g the gravitational acceleration. The difference between Φ_n and Φ_{n-1} will be small if the spring torsion is much larger that the gravitational torque, that is for $\kappa \gg mgl$, in which case the set of difference equations in Eq. (2.1.1) may be approximated by the following partial differential equation (PDE),

$$\frac{\partial^2 \Phi(x,t)}{\partial t^2} - c_0^2 \frac{\partial^2 \Phi(x,t)}{\partial x^2} + \omega_0^2 sin\Phi(x,t) = 0 \ , \tag{2.1.2}$$

with $c_0^2 \equiv \kappa a^2 I^{-1}$ and $\omega_0^2 \equiv mglI^{-1}$ and x is the distance along a line coaxial with the springs. Equation (2.1.2) is the now famous sine-Gordon equation. An entire family of soliton solutions exist which can roughly be classified as being either nonlinear radiation, kinks, or breathers. The nonlinear radiation modes are analogous to the exact Jacobi elliptic function solutions of the single pendulum equation of motion. If the amplitude of these modes are small enough, they reduce to plane waves (torsional sound waves or "phonons") which solve the linearized equation obtained by approximating $\sin\Phi$ by Φ in Eq. (2.1.2). The second class consists of kink and antikink solitons (see Figure 2.2). Kink solutions describe a 0 to 2π twist in the chain whereas the antikinks start from 2π and decrease to 0. The kink or antikink solution of Eq. (2.1.2) is given by

$$\Phi_K(x,t) = 4\arctan(e^{\pm\gamma d^{-1}(x-vt)}) \ , \tag{2.1.3}$$

where v is the velocity of the profile,

$$\gamma = \frac{1}{\sqrt{1 - v^2/c_0^2}} \ , \tag{2.1.4}$$

Figure 2.2: Single kink solution of the sine-Gordon equation.

$$d = \frac{c_0}{\omega_0} \ , \tag{2.1.5}$$

and where the plus sign refers to the kink. The factor of γ appearing in Eq. (2.1.3) is indicative of the fact that the original Lagrangian density

$$\mathcal{L} = \frac{1}{2}\Big(\partial_t \Phi\Big)^2 - \frac{c_0^2}{2}\Big(\partial_x \Phi\Big)^2 - \omega_0^2(1 - \cos\Phi) \ , \tag{2.1.6}$$

has a pseudo-Lorentz invariant form. This invariance enables us to use many of the concepts and relations familiar from relativity. For example, the energy of a kink traveling with velocity v is given by

$$E^{(v)} = E^{(0)}\sqrt{1 - \frac{v^2}{c_0^2}} \ , \tag{2.1.7}$$

where $E^{(0)}$ is the "rest energy"

$$E^{(0)} = M_0 c_0^2 \propto c_0 \omega_0 \ , \tag{2.1.8}$$

$$M_0 = I\frac{\sqrt{2}}{d}\int_0^{2\pi} d\phi \ \sqrt{1 - \cos\phi} \ , \tag{2.1.9}$$

$$= \frac{8I}{d} \ . \tag{2.1.10}$$

The final basic type of solution of the SG equation is the breather which is given by

$$\Phi_B(x,t) = 4\arctan\left(\frac{\tan\nu \sin[(\cos\nu)(t - t_0)]}{\cosh[(\sin\nu)(x - x_0)]}\right) \ . \tag{2.1.11}$$

Figure 2.3: Breather solution of the sine-Gordon equation.

A plot of a breather waveform is shown in Figure 2.3 for the following parameter values:

$$\nu = 1 \quad , \quad x_0 = 0 \quad , \quad t_0 = 1 \; . \tag{2.1.12}$$

Unlike the kink solution, the breather waveform has an envelope which oscillates with time, hence the name breather. In addition to having single kink or breather solutions, there are N soliton solutions which consist of *nonlinear* superpositions of many radiation, kink and breather components. For example, one can find an analytic solution in which at $t = -\infty$ there are N well-separated solitons located to the right of the origin and moving in the negative x direction and M solitons to the left of the origin moving in the positive x direction. If one were to examine this solution for $t \approx +\infty$ one would find the same set of solitons moving to $x = \pm\infty$.

It is indeed quite remarkable that such solutions exist, however one must keep in mind that this is the case only for integrable systems which is not the general situation. More importantly, it is unlikely that real physical systems may be exactly modeled by an integrable equation. Many times, however, soliton-bearing systems serve as a starting point to which perturbations can be added to more closely mimic the real physical system. The addition of such perturbations will certainly modify the propagation of the solitons and will quite likely produce some phonons or radiation. It is therefore of great importance to develop perturbation methods which not only predict the motion of solitons, but also account for any phonons emitted and any effect they may have on the motion of the solitons. Indeed, this interaction between the phonons and the solitons will be the most difficult aspect to capture.

The perturbations which modify the otherwise “straightforward” motion of solitons come in many varieties and again we can make use of the pendulum model for illustrative purposes. Consider for example the effect of an abrupt change of spring constants in the pendulum chain. This effectively changes the limiting speed, c_0, for the soliton and therefore would evidence itself as a term in the Lagrangian density of the form

$$\mathcal{L}_{int} = \frac{1}{2}[\delta c_0(x)]^2 \Phi_x^2(x,t) \ , \tag{2.1.13}$$

where $\delta c_0(x)$ describes the spatial dependence of the perturbation. Instead of coupling to the square of the spatial derivative of the field, one could imagine coupling to the first power, that is a coupling of the form

$$\mathcal{L}_{int} = v(x,t)\Phi_x(x,t) \ , \tag{2.1.14}$$

where in this case we have allowed the perturbation to have an additional time dependence. Since we will always be interested in the integral of the Lagrangian density, it is also reasonable to consider an interaction Lagrangan density which corresponds to integrating Eq. (2.1.14) by parts which would give us

$$\mathcal{L}_{int} = -v'(x,t)\Phi(x,t) \ . \tag{2.1.15}$$

In terms of the pendulum chain, the integrated form in Eq. (2.1.15) is easier to interpret; it corresponds to having a space- and time-dependent torque on the pendulum chain.

These examples in the setting of the pendulum chain are intended to enable us to use physical intuition in our search for a solution to the perturbed problem. However, almost any perturbation which could be introduced in the context of the pendulum chain has an analog in some physical system. For example, the change in the medium manifests itself in the Josephson junction when two such devices are spliced together. The perturbation described by Eq. (2.1.14) occurs in charge-density-wave systems where the derivative of the field represents a local, excess charge density [29]. A rather different type of perturbation which is present in almost all systems is a “damping term” which in terms of the pendulum chain would correspond to submerging the chain in a viscous medium. In addition, the medium would be at some finite temperature and therefore a thermal noise term would have to be added. One could continue with more examples; however, the point is clear: any perturbation method developed should be general enough so that a wide class of such perturbations may be handled.

2.2 Inverse Scattering Perturbation Methods

Having mentioned some of the elegant methods for studying the unperturbed integrable soliton-bearing systems, one might expect that these methods could serve as a basis for perturbation theories. Just such a method was put forth by Keener and McLaughlin [30]. This method treats the interaction of N solitons (on the infinite line) with one another in the presence of weak impurities. This method utilizes the standard method of linearizing about a (nonlinear) zeroth order solution and writing the corrections in terms of a Green function. To ensure that the expansion is valid for times on the order of the inverse perturbation strength, one finds that the unperturbed zeroth order soliton solutions are not a sufficient starting point. However one can show that by allowing the parameters (such as positions and velocities) in these exact solutions to depend slowly on time ("modulate" in time), that the "secularity condition" can be satisified. Using this secularity condition, one derives equations of motion for the soliton position and velocity. Next one solves for the radiation terms using the Green function. To carry out this last step, the inverse scattering transform (IST) is required and herein lies the major drawback of this method. Although the inverse scattering transform is a very powerful and elegant method, it requires a high degree of mathematical sophistication. Even when the calculations are carried out, such as in a study of fluxons in the Josephson junction by McLaughlin and Scott [31], the extraction of physics requires a nontrivial understanding of the inverse scattering transform. However, there are some distinct advantages to this method, one of them being that it applies to "relativistic" motion of solitons. In addition, one can use this method to study multi-soliton waveforms, a feature that is not present in the method discussed in Chapter 3. Yet this strength is also a weakness as it confines us to the study of integrable models.

A similar perturbation theory has been developed by Kaup and Newell [32]. In this theory, one derives modulation equations which to first order are the same as those derived by Keener and McLaughlin. The method is based on the fact that in integrable systems there are an infinite number of conserved quantities and under the influence of weak perturbations these constants will change slowly. Although the first-order equations are equivalent to those obtained by Keener and Mclaughlin, the derivation of Kaup and Newell depends on the inverse method and therefore is somewhat less attractive than the method discussed in the previous paragraph.

The use of conserved quantities was carried a step further by Forest and McLaughlin [33, 34] in their work on the sine-Gordon system *on the finite line* with periodic boundary conditions. Here the use of spectral techniques (for the finite line one uses the inverse spectral transform as opposed to the inverse scattering transform for the infinite line) has led to a much better understanding of the transition to chaos in the damped, driven, sine-Gordon equation [28]. A numerical implementation of these techniques is being carried out by Flesch and Forest [35]

This work is more complex than that outlined above because it involves problems on the finite line. The exact soliton solutions on the finite line are characterized by theta functions on genus-N Riemann surfaces. The calculations essentially require a numerical evaluation of the inverse spectral transform, and although at first glance this task seems to be quite daunting, it can be reduced to performing $2N$ integrals on a genus-N Riemann surface plus solving a system of N coupled ODEs. Again this entire technique is dependent on knowing the canonical transformation to action-angle variables and for the finite line, the problem of finding this transformation has only recently been resolved by Ercolani, Forest and McLaughlin [36] for the sine-Gordon system.

It should be emphasized that the inverse method is essentially a nonlinear analog of the linear Fourier transform and it will be interesting to see how widespread its use becomes in the future. For now we leave the more mathematically based efforts and follow the development of methods which do not depend on the integrable machinery. While such approaches may be inferior when applied to integrable models, they apply to a much broader class.

2.3 The Translation Mode Method

One of the first methods developed to deal with perturbations was presented by Fogel, Trullinger, Bishop and Krumhansl (FTBK) in 1976 [37]. The approach here is one which is often used as a starting point for perturbation theories, namely to decompose the full field $\Phi(x,t)$ into a known zeroth order solution of the system, which is a kink, plus a "phonon" piece . This particular method is restricted to the case in which there is one kink soliton in the system which we denote by $\Phi_K(x,t)$. The basic ansatz for this method is to assume that the solution of the perturbed equation may be written as the sum of the kink plus a "phonon" contribution

$$\Phi(x,t) = \Phi_K(x,t) + \chi(x,t) \ , \tag{2.3.1}$$

where the phonon contribution is assumed to be of the order of the perturbation. To investigate the stability of such an ansatz, one substitutes it into the equation of motion. Since a similar ansatz is the basis for the technique developed in Chapter 3, we consider it in some detail here as applied to the sine-Gordon system. The substitution mentioned above leads to the following equation

$$\ddot{\chi} - \chi'' + \chi \cos \Phi_K = 0 \ . \tag{2.3.2}$$

This equation is further studied in the kink "rest frame" by assuming a harmonic time dependence of the form $\chi(x,t) = f(x)e^{i\omega t}$ which gives us

$$-f'' + f \cos \Phi_K = \omega^2 f \ . \tag{2.3.3}$$

The problem of stability is now reduced to the question of whether the self-adjoint "Schrödinger" operator in Eq. (2.3.3) has any negative eigenvalues ω^2. In the example chosen this question is easily answered since Eq. (2.3.3) is exactly solvable [38] in terms of hypergeometric functions. The spectrum of this operator consists of one zero-frequency discrete state plus continuum states which obey the dispersion relation

$$\omega^2 = 1 + k^2 \ . \tag{2.3.4}$$

Therefore the stability of the ansatz is answered in the affirmative and hence we may go on to consider the significance of the solutions $f_b(x)$ and $f_k(x)$ which label the bound and continuum states respectively.

Since the kink solution is localized in space, it is not surprising to find that the continuum states look very much like plane waves far away from the kink with modification in its vicinity. One can gain similar insight to the bound state solution when one recalls that the original sine-Gordon Lagrangian density is translationally invariant. It would appear that the introduction of a soliton would break this invariance, however one immediately recognizes the zero-frequency bound state as a Goldstone [39] mode which restores translational invariance. Indeed, using the fact that the kink solution $\Phi_K(x)$ satisfies the sine-Gordon equation, one can see that the form which this bound state takes may be given as

$$f_b(x) = \Phi_K'(x) \ . \tag{2.3.5}$$

The addition of a small amount of this bound state has the effect of translating the kink,

$$\Phi_K(x) + \epsilon f_b(x) = \Phi_K(x+\epsilon) + O(\epsilon^2) \ , \tag{2.3.6}$$

and hence the bound state $f_b(x)$ has been termed the translation mode [40].

Now that the linear operator on the left-hand side of Eq. (2.3.3) has been characterized, we may proceed to outline the perturbation method given in Ref. [37]. The phonon field $\chi(x,t)$ is expanded in the complete set $\{f_b(x), f_k(x)\}$ as

$$\chi(x,t) = \phi(t) f_b(x) + \int_{-\infty}^{\infty} dk \ \phi(k,t) f_k(x) \ . \tag{2.3.7}$$

Equations of motion for $\phi(t)$ and $\phi(k,t)$ are then derived, the $\phi(t)$ solution effecting a translation of the kink and the $\phi(k,t)$ producing phonons (radiation and/or a localized shape change in the kink profile).

To understand one of the drawbacks of this method, we consider two cases of a scattering problem in which the kink scatters from $x = -\infty$ to $x = \infty$. In the first case, the initial and final velocities are the same. The net effect of the perturbation is to "phase shift" the kink position, that is the kink position as a function of time differs from the unperturbed situation only by a constant. In this case the translation mode method works well because the perturbation acts on the kink for a short time, and therefore the coefficient of the translation mode

$\phi(t)$ is a well-localized function of time. Compare this result with the case in which the kink's final velocity differs from its initial velocity. Here the difference between the kink position as a function of time in the perturbed and unperturbed cases grows linearly in time. To account for this difference the coefficient of the translation mode must also grow linearly in time. However, the interpretation of the translation mode as effecting a shift in the kink position is approximately valid only for small values of $\phi(t)$. To avoid this problem one must allow the translation-mode coefficient to evolve only for a short time, re-initialize the ODEs, and again calculate a translation-mode coefficient. This secularity (i.e. linear growth in time), along with the fact that the action of the phonons back on the kink motion is difficult to derive, are the major drawbacks of this method. Since many simulations involving a soliton have shown that it acts like an extended particle, it might be expected that one could identify a coordinate which would describe the translation of the soliton without producing secular terms in the perturbation theory.

2.4 Collective Coordinate Methods

Although it was not explicitly pointed out in section 2.2, the method developed by Keener and McLaughlin [30] is one which utilizes collective variables. The positions and velocities of the solitons are allowed to become dynamical variables which obey equations of motion derived from a secularity condition. Another way in which one can make use of collective coordinates is to simply make an ansatz for the field which incorporates parameters which are allowed to depend on time. For example, in the sine-Gordon system we know that exact kink solutions have a parameter x_0 which locates the center of the kink, that is

$$\Phi_K(x,t;x_0) = 4\ \arctan(e^{x-x_0})\ . \tag{2.4.1}$$

By allowing x_0 to depend on time one can define a Lagrangian

$$L(x_0,\dot{x}_0;t) \equiv \int_{-\infty}^{\infty} dx\ \mathcal{L}[\Phi_K(x,t;x_0)]\ , \tag{2.4.2}$$

which by using standard Euler-Lagrange techniques yields a second-order equation for x_0. This method of attack was first used by Rice and Mele as applied to polyacteylene [41]. Results, of course, show a kink translating according to the center of mass coordinate $x_0(t)$. In order to incorporate the fact that the kink behaves like a *deformable* particle, Rice [42] extended this ansatz to include variations of the kink width through the use of a width parameter $l(t)$:

$$\Phi(x,t) = \Phi_K\Big[\frac{x-x_0(t)}{l(t)}\Big]\ . \tag{2.4.3}$$

Proceeding as before, equations of motion are derived for both x_0 and $l(t)$. The equations obtained can be solved for special initial values such as $\dot{l}(0) = 0$ for which he finds that the kink obeys relativistic dynamics. For $\dot{l}(0) \neq 0$ he finds that the velocity of the center of mass of the kink has an oscillatory component superposed on a uniform translation. The existence of "wobbling kink" solutions for the ϕ^4 system has since then been proved by Segur [43]. Similar solutions for the sine-Gordon equation may be constructed, however they have been found to be mildly unstable [43].

Although both of the collective coordinates introduced above appear to be simply parameters of the kink waveform, there is a major difference. If we only include the x_0 coordinate, the ansatz in Eq. (2.4.3) is still a solution of the original field equations. This is a consequence of the translational invariance of the original Lagrangian. In contrast, the only value of l for which Eq. (2.4.3) solves the original field equation is for $l = 1$. Therefore the x_0 coordinate is a more fundamental collective coordinate than the l coordinate. This difference may be further exposed by recalling that the x_0 coordinate is a consequence of the fact that there is a continuous symmetry in the Lagrangian whereas the l coordinate is merely a parameter. For this reason, the l coordinate has been termed a "parametric collective coordinate" [15, 42]. The center of mass collective coordinate is referred to as a "linear collective coordinate" because it can be thought of as arising from the translation mode

$$\Phi_K(x + x_0) \approx \Phi_K(x) + x_0 \Phi'_K(x) \ . \tag{2.4.4}$$

A rather different collective coordinate has been identified by Bergman and co-workers [44]. Their definition uses the fact that since for both topological and non-topological solitons, the derivative of the soliton waveform, which is a measure of the energy density, is a well-localized function in space it therefore gives an indication as to where the soliton is located. Since this derivative is an odd function of x they use as their collective coordinate

$$Q \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} x \Phi_x dx \ , \tag{2.4.5}$$

along with a momentum defined by

$$P \equiv \int_{-\infty}^{\infty} \Pi \Phi_x dx \ , \tag{2.4.6}$$

where Π is the momentum conjugate to Φ. Equations of motion for these newly defined coordinate and momentum variables, which can be shown to be canonically conjugate, are then derived. These equations imply that the soliton behaves as a

Newtonian particle under the influence of an effective potential (after transients, which may be due to turning on the perturbation, have died out). Although the result which states that the soliton behaves as a Newtonian particle confirms previously held beliefs, the method presented says nothing of the phonons emitted and any effect they might have on the soliton. In fact, as defined in Eq. (2.4.5), the coordinate Q includes any phonon effects which might arise. In order to resolve this problem, one would have to clearly identify a soliton and phonon component. Exactly such a separation was acomplished by Tomboulis [45, 46] and independently by Gervais et al. [47]. Since this technique is the basis for the present work, we shall consider it in some detail.

The class of problems to which the method of Tomboulis is applicable can be described by nonlinear Klein-Gordon field theories, that is, field theories which have Lagrangians of the form

$$L = \int_{-\infty}^{\infty} dx \Big\{ \frac{1}{2}\Phi_t^2 - \frac{1}{2}\Phi_x^2 - U(\Phi) \Big\} \ , \tag{2.4.7}$$

where $U(\Phi)$ is a nonlinear potential such as the sine-Gordon, ϕ^4, double quadratic [48] or one of the infinite class of potentials recently found by Trullinger and Flesch [49], to name just a few. The equation of motion for this Lagrangian is given by

$$\Phi_{tt} - \Phi_{xx} + U'(\Phi) = 0 \tag{2.4.8}$$

where x and t are dimensionless space and time variables. The potentials $U(\Phi)$ which are to be studied are those for which Eq. (2.4.8) has exact static kink solutions denoted by $\phi_c(x - X)$ whereas before X was merely a parameter locating the center of the soliton. Again we allow X to become a time-dependent dynamical variable. This would seem to solve one of the problems mentioned above, namely it would identify a pure kink component; however, the phonons have yet to be accounted for. This last problem is solved by making the following transformation

$$\Phi(x,t) = \phi_c(x - X(t)) + \chi(x - X(t), t) \ , \tag{2.4.9}$$

with χ identified as the phonon field. So far Eq. (2.4.9) looks just like several of the ansätze already examined. What sets it apart is the fact that one can find a transformation for the momentum $\Pi_0(x,t)$ conjugate to the field $\Phi(x,t)$

$$\Pi_0(x,t) = \pi(x - X(t)) - \frac{p + \int \pi\chi'}{M_0(1 + \xi/M_0)}\phi_c'(x - X(t)) \ , \tag{2.4.10}$$

$[M_0 \equiv \int \phi_c'^2 \ , \ \xi \equiv \int \chi'\phi_c']$ which makes the entire transformation

$$\{\Phi(x,t), \Pi_0(x,t)\} \longrightarrow \{X(t), p(t), \chi(x,t), \pi(x,t)\} \ , \tag{2.4.11}$$

canonical. (Here, and in the following, integrations over position x are understood to be implicit by integrals signs, unless otherwise indicated. For instance, $\int \chi' \phi_c' \equiv \int_{-\infty}^{\infty} dx\ \chi'(x,t)\phi_c'(x)$.) The X coordinate we have already identified as the kink position coordinate and p is the momentum conjugate to X. Similarly, χ describes the phonon field and π is the momentum conjugate to χ. The part of the transformation given in Eq. (2.4.9) is a very reasonable ansatz while the momentum transformation is what is required for the entire transformation to be canonical; this is also why the argument of the χ field in Eq. (2.4.9) is shifted by X. The rather complex nature of this momentum transformation should tell us that the interaction between the soliton motion and the phonons is indeed quite complicated. One might begin to worry that because the transformation is so nonlinear the equations of motion might not yield a particle-like picture. Although this is indeed something to worry about, we shall show in Chapter 3 that in fact one can derive a Newton's equation for the X variable although in its exact form the force on the "particle" is quite complex.

One of the virtues of the method just outlined is that the transformation can be shown to be *canonical* which is of great benefit when one quantizes the system and when phase space integrals are done. (The Jacobian is unity for a canonical transformation). The existence of a Newton's equation allows us to use intuition from single particle dynamics to guide us in the solution of problems. In addition, having $X(t)$ as a dynamical variable moves the secularity which occurs in the FTBK [37] method to higher order. However, there are of course deficiencies in this method. Even though Tomboulis and Woo [46] have extended this formalism to include multi-soliton waveforms (the degree of difficulty in the actual manipulations needed to implement this more general case increases rapidly with the number of solitons present), it is still restricted to a fairly narrow class of nonlinear problems. An obvious question to ask is whether there are similar transformations available for other classes of soliton-bearing systems.

Although no general method has been proposed to find the proper canonical transformation for an arbitrary nonlinear system, we can point to another example in which one can be found. The nonlinear equation in this case is the double sine-Gordon equation [50]. The potential for a particular version of the double sine-Gordon equation is periodic in 4π with two unequal minima (see Figure 2.4). The 4π kink solution for this system can be viewed as a "bound pair" of successive 2π kinks and is shown in Figure 2.5. As stressed above, one would like to be able to identify certain physically motivated coordinates which describe the system. From Figure 2.5, it is clear what the two relevant coordinates should be in this case, namely a coordinate which fixes the position of the first kink (or the midpoint between the two) and a second which describes the relative displacement of the two kinks. With these coordinates one must look for a canonical transformation

Figure 2.4: Double sine-Gordon potential.

Figure 2.5: The 4π double sine-Gordon kink.

which utilizes them. Such a transformation has been found by Willis and coworkers [51, 52, 53]. In addition they have done some interesting work with discrete versions of the continuum models discussed so far [54, 55]. Therefore the process of identifying pertinent coordinates seems to have some promise and one might wonder to what extent one could push this concept. For example, one could ask to what extent the canonical nature of the transformation is important for classical problems. If one could simply propose a reasonable ansatz based on such coordinates, the applicability of the collective coordinates would greatly expand.

To this end we consider the work of Campbell et al. [15]. In this work the collisions of a ϕ^4 kink and an antikink was investigated via integration of the full PDE. The results showed that, depending on the initial velocity of the incoming kinks, either a bound state was formed which eventually decayed to zero by emission of radiation, or the kinks "resonated with one another" until they separated and finally scattered to $\pm\infty$. The resonance windows observed were quantitatively explained by showing that when the kinks collided there was an exchange of energy from the translational kinetic energy into a shape mode oscillation of the kinks. This shape mode oscillation is little more than a modulation of the kink's width. Here we see another likely candidate for a collective coordinate, namely the width of the kink. Campbell et al. proposed the following ansatz simliar to that used by Rice [42] to study the kink collision

$$\Phi(x,t) = 1 - \phi_c\Big[y_0(x - x_0)\Big] + \phi_c\Big[y_0(x + x_0)\Big] \tag{2.4.12}$$

where x_0 and y_0 are time dependent coordinates. Simulations using this by Flesch and Campbell have so far yielded mixed results which will be discussed in Chapter 7.

2.5 Thermal Fluctuations

So far we have restricted our attention to perturbations which we have been able to describe in terms of a well-defined function $v(x,t)$. Although a great many perturbations fall into this class, it excludes random perturbations caused by thermal fluctuations which are present in all physical systems and are represented by a stochastic function $v(x,t)$ which cannot be given an explicit form but, rather, is characterized only by its correlation functions. Of particular importance are situations in which there is an external field which drives currents. Simple calculations [17] show that at low temperatures the current in Josephson junctions for example is dominated by the motion of kinks. It is therefore important to study the dynamics of solitons under the influence of thermal fluctuations.

One of the first attempts to deal with such perturbations was put forth by Trullinger et al. [56]. Extending a method introduced by Stratanovich [57] and independently by Ambegaokar and Halperin [58] which dealt the motion of a single pendulum, they wrote a multiparticle Fokker-Planck equation for the sine-Gordon chain. By integrating over the momentum degrees of freedom (valid in the large damping limit) a multidimensional Smoluchowski equation was derived. This equation was solved by using a Hartree-like separation ansatz for the distribution function which reduced the problem to a single pendulum problem. The solution of this equation allows one to calculate the average angular velocity of a pendulum. This in turn allows one to calculate a mobility which for low temperatures behaves as $1/T$ with finite-damping corrections given as a power series in the reciprocal damping constant η^{-1} by Lee and Trullinger [59]. Although this result is rather unphysical there is some numerical evidence by Schneider and Stoll [60] which supports a mobility which diverges as $T \to 0$, however their best fit yields a $T^{-3/2}$. We should also note that the reliability of these results has been questioned [61].

A different approach to the problem of thermal fluctuations in the over-damped sine-Gordon system was given by Büttiker and Landauer [61, 62, 63]. This method is based on the calculation of the nucleation rate of kink-antikink pairs which if they are bound weakly enough can be pulled apart by the external field and then contribute to the conduction process. Using these nucleation ideas they calculated a finite zero temperature mobility in contrast with the results of Trullinger et al. [56]. Of course one cannot expect any real physical quantity such as the current to diverge, so the diverging mobility can only be valid for $T > T_0$ for some value of T_0.

An alternate approach for calculating the low temperature mobility was given by Kaup [64]. Using a singular perturbation technique, he calculated the velocity of a heavily damped kink under the influence of a fluctuating force. These results led to a zero temperature mobility which agrees with the value given by Büttiker and Landauer. In addition they found the finite temperature corrections to depend linearly on the temperature.

These radically different results have caused a bit of controversy. Guyer and Miller [65] have compared both methods implemented, pointing out the relevant assumptions made in both. However this has not ended the speculation as evidenced by a comment by Büttiker and Landauer [66] in which they point out some inconsistencies in Guyer and Miller's paper.

A somewhat different method for studying thermal effects on kinks was presented by Wada and Schrieffer [67]. In this work they considered the effect of the collison between a phonon packet and a ϕ^4 kink. They found that to first order the effective force between the kink and the phonons to be purely attractive and that the kink experienced only a phase shift. In addition, it was found that no secondary phonons were created. To introduce the thermal fluctuations they assumed that the phonons were thermally distributed, and then calculated the average displacement of the kink. From this they deduced a "diffusion constant".

I use the quotes here because one usually associates diffusion with the motion of a particle in a viscous medium whereas, as will be shown in Chapter 6, their method predicts that the initial velocity of a kink is not damped to zero.

The same methods used by Wada and Schrieffer were carried to higher order by Ogata, Wada, and coworkers in a series of papers for the ϕ^4 [68, 69], sine-Gordon system [70], and for polyacetylene [71, 72, 73, 74]. Using diagrammatic techniques they found that when one includes terms which are of fourth order in the phonons one finds true dissipation, that is one can show that a fluctuation-dissipation theorem holds. However, as in the work of Wada and Schrieffer, they did not include any explicit coupling to an external heat bath. They merely assumed that somehow the phonons were described by some distribution function. We shall show in Chapter 6 that their choice of distribution functions is in fact the correct one to use in lowest order *if an explicit coupling to a heat bath is also included.* Without such a coupling, some very important physics is missed, namely that to lowest order the kink behaves just like a Brownian particle. This result is recovered when a collective-coordinate approach is implemented. Furthermore, we find that the thermal fluctuations have the effect of adding temperature-dependent corrections to the mass and diffusion constant.

Chapter 3

Collective-Coordinate Perturbation Theory

Having reviewed many of the perturbation theories used to study soliton dynamics, we develop a new method based on a canonical transformation developed by Tomboulis. This transformation identifies a "center of mass" coordinate $X(t)$ which is found to satisify a Newtonian equation of motion (to lowest order)

$$M_0 \ddot{X} = F(\dot{X}, t) \ ,$$

adding to the existing evidence [30, 31, 32, 37, 42, 44] which indicates that the kink does indeed behave like an extended Newtonian particle (for low velocities). The extended nature of this particle becomes apparent when the exact form of the force on the kink is examined. Before deriving this force, we quickly review some of the important facts about the small oscillations about nonlinear Klein-Gordon kinks.

3.1 Small Oscillations

In this section we briefly review the main features of solutions to the nonlinear Klein-Gordon class of field theories and the canonical transformation which forms the basis for our perturbation theory. The single-kink solutions to the wave equations along with small oscillations about these kinks will be described. The various quantities described in this section are collected in Table I for the sine-Gordon, ϕ^4, and double-quadratic potentials (this table corrects some errors in Table 3.1 of Ref. [75] and a similar error in Eq. 4.16b in Ref. [76]).

The general nonlinear Klein-Gordon Lagrangian we consider has the form

$$L = \int_{-\infty}^{\infty} dx \Big\{ \frac{1}{2}\Phi_t^2 - \frac{1}{2}\Phi_x^2 - U(\Phi) \Big\} \ , \tag{3.1.1}$$

Table 3.1: Various quantities for the ϕ^4, SG and DQ systems

where x and t are dimensionless space and time variables and $U(\phi)$ is the nonlinear potential with at least two degenerate minima. The nonlinear wave equation satisified by $\Phi(x,t)$ is

$$\Phi_{tt} - \Phi_{xx} + U'(\Phi) = 0 \ , \tag{3.1.2}$$

where the prime on $U(\Phi)$ denotes a derivative with respect to Φ. Static single-kink solutions, $\phi_c(x)$, of Eq. (3.1.2) may be obtained by direct integration with the boundary conditions

$$\frac{d\phi_c(x)}{dx}\Big|_{x=\pm\infty} = 0 \ , \tag{3.1.3}$$

The static kink (+) and antikink (-) solutions are given by

$$x = \pm\frac{1}{\sqrt{2}}\int_{\phi_c(0)}^{\phi_c(x)} \frac{d\phi}{\sqrt{U(\phi)}} \ , \tag{3.1.4}$$

Moving solutions can be obtained by a Lorentz boost.

The equation governing the small oscillations about the static kink waveform is obtained by substituting

$$\Phi(x,t) = \phi_c(x) + \psi(x,t) \ , \tag{3.1.5}$$

into Eq. (3.1.2) and linearizing in ψ:

$$\psi_{tt} - \psi_{xx} + \psi U''[\phi_c(x)] = 0 \ . \tag{3.1.6}$$

Here $U''[\phi_c(x)]$denotes the second derivative of $U(\phi)$ with respect to ϕ evaluated for $\phi = \phi_c(x)$. Writing ψ as

$$\psi(x,t) = f(x)e^{i\omega t} \ , \tag{3.1.7}$$

leads to the following eigenvalue equation:

$$-f_{xx} + U''[\phi_c(x)]f = \omega^2 f \ . \tag{3.1.8}$$

Due to the localized nature of the kink waveform $\phi_c(x)$, the function $U''[\phi_c(x)]$ varies mainly in the region of the kink center (assumed to be at $x = 0$) and approaches a constant (taken to be unity) far from the kink center:

$$U''[\phi_c(x)] \xrightarrow[|x|\to\infty]{} 1 \ . \tag{3.1.9}$$

Moreover, the function $U''[\phi_c(x)]$ has a minimum at x=0 such that

$$U''[\phi_c(0)] < 0 \ . \tag{3.1.10}$$

From these properties, we see that there exists a close analogy between Eq. (3.1.8) and the Schrödinger equation for a "particle" moving in a one-dimensional "potential well", $U''[\phi_c(x)]$. The "bound state(s)" and "continuum" states for this potential are of fundamental importance for statistical mechanics phenomenologies [76], perturbation theories for kink dynamics [76, 37], and quantization procedures for kink states [77, 45, 47, 78, 79, 80, 81].

Since the Lagrangian (3.1.1) possesses translational invariance, the spectrum of the small oscillations about the single kink must contain a zero-frequency ($\omega = 0$) "translation" mode (Goldstone mode) which restores the translational invariance broken by the introduction of the kink. In addition to this translation mode there may be other discrete eigenvalues ("bound states") with frequencies between 0 and 1. These solutions, denoted by $f_{b,i}(x)$, correspond to "internal" oscillation modes in which the kink undergoes a harmonically varying shape change localized about the kink center. We denote these bound-state eigenfrequencies by $\omega_{b,1} \ldots \omega_{b,N}$ where N is the total number of bound states. The lowest of these is $\omega_{b,1} = 0$ since all other $\omega_{b,i}^2$ must be non-negative in order for the kink to be stable against small oscillations.

In addition to the bound states, there exist continuum states (continuous spectra) which are labelled by a wavevector k. These states have eigenvalues ω_k^2 given by

$$\omega_k^2 = 1 + k^2 \ . \tag{3.1.11}$$

which is precisely the dispersion relation for small oscillations in the absence of kinks.

The continuum states together with the bound-states form a complete set and satisfy the completeness relation,

$$\sum_{i=1}^{N} f_{b,i}^*(x) f_{b,i}(x') + \int_{-\infty}^{\infty} dk f_k^*(x) f_k(x') = \delta(x - x') \ . \tag{3.1.12}$$

and the following orthogonality relations:

$$\begin{aligned} \int_{-\infty}^{\infty} dx f_{b,n}(x) f_{b,m}(x) &= \delta_{m,n} \ , \\ \int_{-\infty}^{\infty} dx f_k^*(x) f_{k'}(x) &= \delta(k - k') \ , \\ \int_{-\infty}^{\infty} dx f_k(x) f_{b,n}(x) &= 0 \ . \end{aligned} \tag{3.1.13}$$

In the case in which $\phi_c'(x)$ is symmetric, $U''[\phi_c(x)]$ is also symmetric and therefore the continuum states may be chosen to have definite parity (if desired):

$$f_k(-x) = \pm f_{-k}(x) = \pm f_k^*(x) \ . \tag{3.1.14}$$

In addition, the following identity has been recently found [82]

$$\sum_{i=2}^{N} \frac{1}{\omega_{b,i}^2} f_{b,i}^*(x) \int\limits_{-\infty}^{\infty} dy f_{b,i}(y)\phi_c''(y) + \int\limits_{-\infty}^{\infty} dk \ \frac{1}{\omega_k^2} f_k^*(x) \int\limits_{-\infty}^{\infty} dy f_k(y)\phi_c''(y) = \frac{1}{2} x\phi_c'(x) \ , \tag{3.1.15}$$

which can be readily proved by applying $-\partial^2/\partial x^2 + U''[\phi_c(x)]$ to both sides of Eq. (3.1.15).

Having illustrated the complete set of states associated with the linear operator given in Eq. (3.1.6), one might conclude that all of the relevant solutions of Eq. (3.1.6) have been found. This is not the case as has been pointed out in some recent work of Magyari and Thomas [83]. In searching for solutions of Eq. (3.1.6) we assumed a harmonic time dependence. However in general we should make the separation of variables ansatz

$$\psi = Q(t)f(x) \ . \tag{3.1.16}$$

Substituting this separation ansatz into Eq. (3.1.6) we obtain the following equation for $Q(t)$:

$$Q''(t) + \lambda Q(t) = 0 \ , \tag{3.1.17}$$

where λ is the separation constant. For $\lambda \neq 0$ we do indeed find a harmonic time dependence for $Q(t)$, however for $\lambda = 0$ there exists another solution which is linear in time

$$Q(t) = at + b \ . \tag{3.1.18}$$

Therefore we find that we have a degeneracy of the zero frequency eigenvalue. Just as the original zero frequency can be interpreted as having the effect of translating the kink in space, the second solution, termed the "defective degeneracy" [83], has the effect of inducing an infinitesimal velocity change in the kink. To see this we simply add the second solution to a stationary kink

$$\phi_c(x + \epsilon t) \approx \phi_c(x) + \epsilon t\phi_c'(x) \ . \tag{3.1.19}$$

The physical significance of this defective degeneracy can be further illustrated by considering the effects of an additional damping term $\eta\Phi_t$ to Eq. (3.1.2). Using the same separation ansatz we obtain the following equation for $Q(t)$

$$Q''(t) + \eta Q'(t) + \lambda Q(t) = 0 \ . \tag{3.1.20}$$

Again one can assume a harmonic time dependence

$$Q(t) = e^{-i\omega_{1,2}t} \ , \tag{3.1.21}$$

with $\omega_{1,2}$ given by

$$\omega_{1,2} = \pm\sqrt{\lambda - \frac{1}{4}\eta^2} - \frac{1}{2}i\eta \ . \tag{3.1.22}$$

Now the eigenvalue $\lambda = 0$ is no longer degenerate since in this case we obtain $\omega = 0$ (Goldstone mode) and $\omega = -i\eta$. Therefore with the addition of damping, the defective degeneracy of the $\lambda = 0$ eigenvalue is lifted by the occurence of the "relaxation mode"

$$Q(t) = e^{-\eta t} \ , \tag{3.1.23}$$

which describes the deceleration of an infinitesimally slowly moving kink to a shifted ($\phi_c'(x)$ still shifts the kink) static kink. This "degree of freedom" is actually accounted for by the kink velocity coordinate $\dot{X}(t)$ which is introduced in the next section.

3.2 The Collective Coordinate and the Canonical Transformation

As mentioned in Chapter 2, a transformation to a set of variables in which one can easily identify a kink coordinate would be of great utility when one describes the motion of a kink. Such a transformation has been found [45, 47] for *unperturbed* nonlinear Klein-Gordon field theories. This transformation decomposes the full field $\Phi(x,t)$ into a classical kink solution $\phi_c(x)$ whose center translates according to the dynamical variable $X(t)$ plus a "radiation" field $\chi(x,t)$

$$\Phi(x,t) = \phi_c(x - X(t)) + \chi(x - X(t), t) \tag{3.2.1}$$

The momentum conjugate to the field $\phi(x,t)$ is also decomposed into a soliton component plus a radiation field

$$\Pi_0(x,t) = \pi(x - X(t), t) - \frac{p + \int \pi\chi'}{M_0(1 + \xi/M_0)}\phi_c'(x - X(t)) \ , \tag{3.2.2}$$

where $M_0 \equiv \int \phi_c'\phi_c'$ and $\xi \equiv \int \chi'\phi_c'$. The prime denotes differentiation with respect to the argument and unless otherwise specified, all integrals denote one-dimensional integrals over x.

Having made the transformation

$$\{\Phi(x,t), \Pi_0(x,t)\} \to \{X(t), p(t), \chi(x,t), \pi(x,t)\} \ , \tag{3.2.3}$$

one notices that the number of degrees of freedom are not conserved, that is, on the left-hand side of Eq. (3.2.3) we have two full field degrees of freedom whereas on the right-hand side we have two full field degrees of freedom plus two discrete degrees of freedom. To remedy this situation, we must impose the following two constraints

$$
\begin{aligned}
\int_{-\infty}^{\infty} dx\ \chi(x,t)\phi_c'(x) &= 0\ , \\
\int_{-\infty}^{\infty} dx\ \pi(x,t)\phi_c'(x) &= 0\ .
\end{aligned} \tag{3.2.4}
$$

The first of these constraints has the interpretation that the ψ field cannot have a term proportional to the translation mode, that is, the effect of the ψ field cannot cause the kink to translate. This is a very reasonable constraint since we have a dynamical variable whose only purpose is to translate the kink. The second of the constraints has a similar interpretation.

This transformation is not typical due to the presence of the constraints. To show that it is a canonical transformation, one must resort to the Dirac formalism for constrained systems [84]. Usually when one deals with constrained systems, the constraints cannot be used until all of the Poisson brackets have been taken, that is, the equalities in Eqs. (3.2.4) are "weak equalities". The Dirac formalism makes these equalities strong by modification of the brackets (Dirac brackets). For this particular transformation the brackets are

$$
\Big\{\chi(x,t),\pi(y,t)\Big\} = \delta(x-y) - \frac{1}{M_0}\phi_c'(x)\phi_c'(y)\ , \tag{3.2.5}
$$

$$
\Big\{X,p\Big\} = 1\ , \tag{3.2.6}
$$

with all remaining brackets vanishing. Using these brackets one can verify that the brackets in terms of the original variables satisfy the standard relations, that is

$$
\Big\{\Phi(x,t),\Phi(y,t)\Big\} = \Big\{\Pi_0(x,t),\Pi_0(y,t)\Big\} = 0\ . \tag{3.2.7}
$$

$$
\Big\{\Phi(x,t),\Pi_0(y,t)\Big\} = \delta(x-y)\ , \tag{3.2.8}
$$

In what follows, every time a bracket appears it is meant to indicate a Dirac bracket.

We can gain further insight into the transformation by examining the form which some of the energy-momentum tensor elements take in terms of the new variables. First we consider the Hamiltonian

$$
\begin{aligned}
H &= \int T_{00} \\
&= \int \left\{ \frac{1}{2}\Pi_0^2 + \frac{1}{2}\Phi'^2 + U(\Phi) \right\}\ , \\
&= M_0 + \frac{1}{2M_0}\frac{(p+\int \pi\chi')^2}{(1+\xi/M_0)^2} + \int \mathcal{H}_f\ ,
\end{aligned} \tag{3.2.9}
$$

where

$$\mathcal{H}_f = \frac{1}{2}\pi^2(x,t) + \frac{1}{2}\chi'^2(x,t) + V(\chi,\phi_c) \ , \tag{3.2.10}$$

$$V(\chi,\phi_c) = U(\phi_c+\chi) - \chi(x,t)U'(\phi_c) - U(\phi_c) \ , \tag{3.2.11}$$

where primes denote differentiation with respect to the argument and repeated use of

$$\phi_c'' = U'(\phi_c) \ , \tag{3.2.12}$$

and

$$\frac{1}{2}(\phi_c')^2 = U(\phi_c) \ , \tag{3.2.13}$$

has been made. Given the Hamiltonian in terms of the new variables, one can derive the equations of motion for the dynamical variables. In particular we find that the equation for X is given by

$$\dot{X} = \frac{p + \int \pi\chi'}{M_0(1+\xi/M_0)^2} \tag{3.2.14}$$

Using this equation of motion for X we can rewrite the Hamiltonian as

$$H = M_0 + \frac{1}{2}M_0(1+\xi/M_0)^2\dot{X}^2 + \int \mathcal{H}_f \ . \tag{3.2.15}$$

In this form we see that H almost decouples into a kink contribution and a phonon contribution. The term which prevents this decoupling can be understood to be a renormalization of the mass M_0. This coupling represents the interaction of the phonons back on the kink and is one the most interesting aspects of this method.

Next we turn our attention to the total momentum of the system

$$\begin{aligned}
P &\equiv \int T_{01} = -\int T^{01} \ , && (3.2.16)\\
&= \int \Pi_0(x,t)\Phi'(x,t) \ , && (3.2.17)\\
&= \int \pi(x-X,t)\Big[\phi_c'(x-X) + \chi'(x-X,t)\Big] \\
&- \frac{p+\int\pi\chi'}{M_0(1+\xi/M_0)}\int\Big[\phi_c'(x-X)\chi'(x-X,t) + \phi_c'(x-X)\phi_c'(x-X)\Big] \\
& && (3.2.18)\\
&= \int \pi\chi' - \frac{p+\int\pi\chi'}{M_0(1+\xi/M_0)}(M_0+\xi) && (3.2.19)\\
&= p \ . && (3.2.20)
\end{aligned}$$

From this we see that the variable p actually represents the total momentum of the system and not the kink momentum, even though it is conjugate to $X(t)$. It might appear that this would be rather inconvenient when one wishes to interpret the solutions to the equations of motion. This is not the case since in the following section we derive a second order equation for X. However it does present difficulties when we want to fix kink degrees of freedom in the Fokker-Planck method to be developed in Chapter 6. This problem can be avoided by using a transformation in which the momentum conjugate to the center of mass variable X is the kink momentum. The transformation for which p is the kink momentum is given by

$$\Phi(x,t) = \phi_c(x - X(t)) + \chi(x,t) \tag{3.2.21}$$

$$\Pi_0(x,t) = \pi(x,t) - \frac{p + \int \pi\chi'}{M_0(1+\xi/M_0)}\phi_c'(x - X(t)) \ , \tag{3.2.22}$$

with the constraints

$$\begin{aligned} \int_{-\infty}^{\infty} dx \ \chi(x,t)\phi_c'(x-X) &= 0 \ , \\ \int_{-\infty}^{\infty} dx \ \pi(x,t)\phi_c'(x-X) &= 0 \ . \end{aligned} \tag{3.2.23}$$

To complete the transformation the Dirac brackets must be presented. The bracket of χ with π is the same as before but the brackets of the phonon variables χ and π with the momentum p become

$$\Big\{\chi(x,t), p\Big\} = 1 - \frac{\xi}{M_0}\phi_c'(x-X) \ , \tag{3.2.24}$$

$$= 1 - \mathcal{P}_{\phi_c}\chi'(x-X) \tag{3.2.25}$$

$$\Big\{\pi(x,t), p\Big\} = 1 - \frac{\phi_c'(x-X)}{M_0}\int_{-\infty}^{\infty} dx \ \phi_c'(x-X)\pi'(x,t) \ , \tag{3.2.26}$$

$$= 1 - \mathcal{P}_{\phi_c}\pi'(x-X) \ , \tag{3.2.27}$$

with all other brackets zero. In the last step we have introduced the "translation-mode" projection operator $\mathcal{P}_{\phi_c}$ defined by

$$\mathcal{P}_{\phi_c}G(x,t) = \frac{\phi_c'(x)}{M_0}\int \phi_c'(x)G(x,t) \ . \tag{3.2.28}$$

This operator projects out that piece of any function which "overlaps" with the translation mode $\phi_c'(x)$.

In the actual calculation of the equations of motion one does not gain any advantage with either of the two brackets. The second transformation has the advantage that p is the kink momentum while the first, which is the one which will be implemented in the following chapters, has the virtue that the phonon field translates with the kink center of mass. This is especially useful when the interaction of the kink with the perturbation results in a permanent distortion of the kink waveform.

Finally we note that with the additional definition of a Lorentz boost generator

$$L = \int xT_{00} \; , \tag{3.2.29}$$

Tomboulis has shown [45] that the three operators H, P, and L form a Poincaré algebra,

$$\begin{aligned} \{H, P\} &= 0 \\ \{L, P\} &= H \\ \{L, H\} &= P \; , \end{aligned} \tag{3.2.30}$$

and therefore the unperturbed transformation preserves the Lorentz invariance evident in the Lagrangian.

3.3 The Perturbed System

The types of perturbations which we study have interaction Hamiltonians which may be written in the form

$$H_{int} = -\int_{-\infty}^{\infty} dx \; v(x,t) \; F[\Phi(x,t), \Phi_x(x,t)] \; , \tag{3.3.1}$$

where $v(x,t)$, assumed small in magnitude, denotes the space and time dependence of the perturbation and $F[\Phi(x,t), \Phi_x(x,t)]$ tells us how the perturbation couples to the field. The case in which the coupling function F is linear in the field and $v(x,t) = \delta(x - x_0)$ could be physically realized in terms of the pendulum chain if one of the pendula experienced a uniform external torque. Similarly for the pendulum chain, if $F = \Phi_x^2$ and $v(x,t) = \theta(x - x_0)$, the perturbation may be thought of as arising from an abrupt change in the spring constant of the chain. The general form of the perturbation (3.3.1) should allow many other types of perturbations to be examined, some of which will be presented in Chapter 5.

The aim of the perturbation theory is of course to study its influence on the kink. It should be kept in mind that even without the presence of a kink the perturbation influences the system. For example, if the perturbation is a torque on one of the pendula as mentioned above, the field in the vicinity of the applied torque will be modified as shown in Figure 3.1 This deformation will be present with or without the kink. If the kink scatters off of this perturbation,

Figure 3.1: Response of the sine-Gordon pendulum chain to a constant torque on a single pendulum

long before and after the scattering event the field in the region of the torque will be as shown in Figure 3.2 (neglecting any emitted phonons). The transformation described in the previous section could account for this feature through the χ field, however this is unattractive since then $\chi(x, \pm\infty)$ would be nonzero making the boundary conditions more difficult to deal with. Indeed, if this background response is not included from the outset, the field evolves in such a way as to "build up" this response and, in the process, the kink dynamics can appear [85] to be non-Newtonian. It is clear that one would like to take care of this deformation from the start and, in doing so, Newtonian dynamics is recovered. We accomplish this by introducing the "background" field $\psi_0(x,t)$ and modifying the canonical transformation to include it as follows

$$\Phi(x,t) = \phi_c[x - X(t)] + \psi[x - X(t), t] + \psi_0(x,t) \ , \tag{3.3.2}$$

$$\Pi_0(x,t) = \pi[x - X(t)] - \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)}\phi_c'[x - X(t)] - \dot{\psi}_0(x,t) \ , \tag{3.3.3}$$

where M_0 and ξ are still defined by

$$M_0 = \int \phi_c'\phi_c' \ , \tag{3.3.4}$$

$$\xi = \int \psi'\phi_c' \ , \tag{3.3.5}$$

and the constraints are given by

$$\int dx\ \phi_c'(x)\psi(x,t) \;=\; 0 \tag{3.3.6}$$

$$\int dx\ \phi_c'(x)\pi(x,t) \;=\; 0\ . \tag{3.3.7}$$

The ψ_0 term in Eq. (3.3.2) represents the response of the field to the perturbation *in the absence of a kink* and obeys the following equation:

$$[\partial_{tt} - \partial_{xx}]\psi_0(x,t) + \psi_0 U'(\psi_0) - F_{10}[\psi_0,\psi_0']v(x,t) + \frac{d}{dx}(v(x,t)F_{01}[\psi_0,\psi_0']) = 0\ , \tag{3.3.8}$$

with F_{ij} defined by

$$F_{ij} \equiv \frac{\partial^{i+j}F[\Phi,\Phi_x]}{\partial\Phi^i\partial\Phi_x^j}\ . \tag{3.3.9}$$

The field decomposition given in Eq. (3.3.2) is perhaps best illustrated with an example. Consider the “torqued pendulum” perturbation mentioned above with the kink scattering from $X = -\infty$ to $X = \infty$. In Figure 3.2 we show the field for times long before and after the scattering takes place. For $t = -\infty$ the kink has not yet interacted with the perturbation and therefore the field consists of the kink plus the background deformation. For large positive times the kink has scattered off of the perturbation and in the process emitted some phonons. These phonons are described by the ψ field while the ψ_0 field still accounts for the deformation in the region of the applied torque.

It has been shown [45] that Eqs. (3.3.2) and (3.3.3) specify a canonical transformation when no perturbation is present, that is for $\psi_0 = 0$ and $v(x,t) = 0$. That Eqs. (3.3.2) and (3.3.3) along with the constraints in Eqs. (3.3.6) and (3.3.7) still form a canonical transformation in the presence of a perturbation can be proved as follows. For no perturbation, Eqs. (3.3.2) and (3.3.3) are a point transformation of equations (3.2.1) and (3.2.2) and therefore the transformation is still canonical. The addition of a perturbing piece to the Hamiltonian has no effect since the canonical nature of the transformation depends only on the transformation equations and not on the Hamiltonian [86].

With the canonical transformation in hand, we may proceed to derive the equations of motion for the dynamical variables by using the Dirac-bracket formalism for constrained systems [84]. As in the previous section, the nonzero brackets for our system are

$$\{\psi(x,t),\pi(y,t)\} \;=\; \delta(x-y) - \frac{\phi_c'(x)\phi_c'(y)}{M_0}\ , \tag{3.3.10}$$

$$\{X(t),p(t)\} \;=\; 1 \tag{3.3.11}$$

Figure 3.2: The various contributions to the field for the "torqued pendulum" perturbation. The solid line represents the kink contribution, the dashed line the background field ψ_0 and the dotted line the phonon portion ψ.

The bracket in Eq. (3.3.10) may be interpreted as a projection operator when it occurs under an integral sign which is always the case when the equations of motion are derived. For example, consider the following operation involving an arbitrary functional $G[\pi(y,t)]$ of the momentum field:

$$\begin{aligned}
&\int dx\{\psi(x,t), G(\pi(y,t))\} \\
&= \int dx G'(\pi(y,t))\{\psi(x,t),\pi(y,t)\} && (3.3.12)\\
&= G'(\pi(x,t)) - \frac{\phi_c'(x)}{M_0}\int \phi_c'(x)G'(\pi(x,t)) && (3.3.13)\\
&= (1-\mathcal{P}_{\phi_c})G'(\pi(x,t)) \ . && (3.3.14)
\end{aligned}$$

Given the brackets in Eqs. (3.3.10) and (3.3.11) , we may derive the equations of motions by taking the Dirac bracket of the dynamical variables with the Hamiltonian. Using the fact that the Hamiltonian in terms of the original variables is given by

$$H = \frac{1}{2}\int_{-\infty}^{\infty} dx\ \left[\Pi_0^2(x,t) + \Phi'^2(x,t) + U[\Phi]\right] + H_{int}\ , \tag{3.3.15}$$

we write the Hamiltonian in terms of the new variables as

$$H = H_0 + H_{\psi_0} + H_{int}\ , \tag{3.3.16}$$

where

$$H_0 = M_0 + \frac{1}{2M_0}\frac{(p+\int\pi\psi')^2}{(1+\xi/M_0)^2} + \int H_f\ , \tag{3.3.17}$$

$$H_f(x,t) = \frac{1}{2}\pi^2(x,t) + \frac{1}{2}\psi'^2(x,t) + V(\psi,\phi_c)\ , \tag{3.3.18}$$

and

$$V(\psi,\phi_c) = U(\phi_c+\psi) - \psi(x,t)U'(\phi_c) - U(\phi_c)\ . \tag{3.3.19}$$

H_{int} is given in Eq. (3.3.1) and H_{ψ_0} is defined by

$$\begin{aligned}
H_{\psi_0} &= -\pi[x-X(t),t]\dot{\psi}_0'(x,t) + \frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)}\phi_c'[x-X(t)]\dot{\psi}_0(x,t) \\
&+ \psi'[x-X(t),t]\psi_0'(x,t) + \phi_c'[x-X(t)]\psi_0'(x,t) + \Delta U\ , && (3.3.20)
\end{aligned}$$

with

$$\Delta U = U[\phi(x)+\psi(x,t)+\psi_0(x+X(t),t)] - U[\phi(x)+\psi(x,t)]\ . \tag{3.3.21}$$

The calculation of the equations of motion for X, p, ψ, π is straightforward but tedious and is therefore relegated to Appendix A.

Since we are most interested in the kink center of mass motion, it is useful to derive a second order equation for the kink center of mass variable $X(t)$. Using Eq. (A.23) from Appendix A we have

$$\begin{aligned} M_0\ddot{X} &= \frac{1}{(1+\xi/M_0)}\Big\{-\int v(x,t)\Big[\phi_c'(x-X)F_{10}[\Phi,\Phi_x]+\phi_c''(x-X)F_{01}[\Phi,\Phi_x]\Big] \\ &+ \int\Big[\ddot{\psi}_0(x,t)-\psi_0''(x,t)\Big]\phi_c'(x-X)+\int\phi_c'(x-X)U'[\Phi(x,t)] \\ &+ (1+\dot{X}^2)\int\psi'\phi_c''-2\dot{X}\int\pi'\phi_c'+2\dot{X}\int\phi_c'(x)\dot{\psi}_0'(x+X,t)\Big\}\ . \end{aligned} \tag{3.3.22}$$

where Φ is understood to mean $\Phi(x,t)$. Since we have not yet made any approximations, Eq. (3.3.22) is *exact* and states that the kink center of mass variable $X(t)$ obeys Newton's law. The "force" that the kink experiences, that is the right-hand side of Eq. (3.3.22), has several interesting properties. First, it includes terms which depend on the radiation field $\psi(x,t)$ and therefore the equations that must be solved are really a set of integro-differential equations which are most easily solved perturbatively. Physically, the presence of ψ in the kink equations means that any phonons produced by the propagation of the kink in the perturbed system in turn affect the kink's motion. The second interesting feature of the "force" on the kink is that one of the terms is proportional to the square of the kink velocity, that is, there is a "dissipative" term in the center of mass equation of motion. Because we started with a Hamiltonian system, this "dissipative" term cannot represent a real loss of energy. Rather, this term represents a transfer of energy between the kink center of mass motion and the radiation field.

One is tempted to interpret the term which is linear in $\dot{X}$ as also representing a transfer of energy. However, further examination of Eq. (3.3.22) indicates that this term is actually part of the inertia of the kink. To see this we make use of Eq. (A.13) of Appendix A to replace the $\pi'(x,t)$ term in Eq. (3.3.22) by an equivalent expression in terms of the ψ and ψ_0 fields:

$$\int\pi'\phi_c' = \int\dot{\psi}'\phi_c' - \dot{X}\int\psi''\phi_c' + \int\dot{\psi}_0'(x+X,t)\phi_c'(x)\ . \tag{3.3.23}$$

Substitution of this expression in to Eq. (3.3.22) yields

$$\begin{aligned} M_0\ddot{X} &= \frac{1}{(1+\xi/M_0)}\Big\{-\int v(x,t)\Big[\phi_c'(x-X)F_{10}[\Phi,\Phi_x]+\phi_c''(x-X)F_{01}[\Phi,\Phi_x]\Big] \\ &+ \int\Big[\ddot{\psi}_0(x,t)-\psi_0''(x,t)\Big]\phi_c'(x-X)+\int\phi_c'(x-X)U'[\Phi(x,t)] \\ &+ (1-\dot{X}^2)\int\psi'\phi_c''-2\dot{X}\int\dot{\psi}'\phi_c'\Big\}\ . \end{aligned} \tag{3.3.24}$$

Next we move the term linear in $\dot{X}$ to the left-hand side of the equation and multiply by $1+\xi/M_0$ which allows us to write

$$\begin{aligned}
&\frac{d}{dt}\Big[M_0(1+\xi/M_0)^2\dot{X}\Big] \\
&= (1+\xi/M_0)\bigg\{-\int v(x,t)\Big[\phi_c'(x-X)F_{10}[\Phi,\Phi_x]+\phi_c''(x-X)F_{01}[\Phi,\Phi_x]\Big] \\
&+ \int\Big[\ddot{\psi}_0(x,t)-\psi_0''(x,t)\Big]\phi_c'(x-X)+\int\phi_c'(x-X)U'[\Phi(x,t)] \\
&+ (1-\dot{X}^2)\int\psi'\phi_c''\bigg\}\ , \qquad (3.3.25)
\end{aligned}$$

where we have made use of the fact that

$$\dot{\xi} = \int\dot{\psi}'\phi_c'\ . \qquad (3.3.26)$$

Equation (3.3.25) is nothing more that Newton's law for a particle with time-dependent mass

$$M = M_0(1+\xi/M_0)^2\ . \qquad (3.3.27)$$

Therefore we see that one of the effects of the phonon field is to renormalize the mass of the kink. This feature of the phonon field has already been noted in the quantized theories for the unperturbed system [47]. The interpretation of the left-hand side of Eq. (3.3.25) as being the time derivative of the kink momentum is verified by examining the equation for $\dot{X}$ derived in Appendix A. Rewriting Eq. (A.11) we have

$$M_0(1+\xi/M_0)^2\dot{X} = p+\int\pi\psi'+(1+\xi/M_0)A(X,t)\ , \qquad (3.3.28)$$

which states that the kink momentum equals the total momentum of the system p minus the momentum of the phonon field ($-\int\pi\psi'$) minus a momentum term due to the background.

Equation (3.3.22) was derived by using the fact that Eqs. (3.3.2) and (3.3.3) plus the constraints form a canonical transformation and therefore the Dirac bracket of the dynamical variables with the Hamiltonian yields the equations of motion. An alternate method is available which uses the fact that in Eqs. (3.3.2) and (3.3.3) we have a transformation in which the old coordinates are expressible in terms of the new coordinates and therefore, one can derive the equations of motion simply by taking the appropriate derivatives of Eqs. (3.3.2) and subsituting them into Eq. (3.1.2). In fact, we can generalize Eq. (3.1.2) by including a phenomenological damping term of the form

$$\epsilon\dot{\Phi}(x,t)\ .$$

Unlike the "damping" terms in Eq. (3.3.22), this term is truly dissipative and may be envisioned as arising from coupling the system to a heat bath.

Although substitution of Eq. (3.3.2) into Eq. (3.1.2) (see Appendix B) yields the correct equations of motion more quickly and with less work than using the canonical formalism, this in no way means that we can abandon the canonical transformation. A major reason for this is that the canonical structure allows us to use the standard prescription of promoting canonical variables to operators and the Poisson bracket to commutators when we wish to quantize the system [45, 47]. In addition, when one works with phase space integrals as is the case in Fokker-Planck (see Chapter 6) or Boltzmann approaches, having a canonical transformation preserves the phase space volume element (for our transformation which involves constraints, the Jacobian is actually the product of the delta functions whose arguments are exactly the constraints in Eqs. (3.2.4) [47]).

3.4 The Perturbation Expansion

We now turn our attention to the task of obtaining an approximate solution of Eq. (3.3.24) as a perturbation series. We assume that the perturbation $v(x,t)$ is proportional to some small parameter which we denote by λ. Since we are mainly interested in the motion of the kink center of mass, we begin by expanding Eq. (3.3.2). For these purposes, we assume that $v(x,t)$, $\psi(x,t)$ and $\psi_0(x,t)$ are all of order λ. To obtain the expansion of Eq. (3.3.24) through order λ^2, we make use of the following Taylor series

$$F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)] = \frac{\partial F(\phi_c,\phi_c')}{\partial\phi_c} + \chi(x,t)\frac{\partial^2 F(\phi_c,\phi_c')}{\partial^2\phi_c^2} + \chi'(x,t)\frac{\partial^2 F(\phi_c,\phi_c')}{\partial\phi_c'\partial\phi_c} \tag{3.4.1}$$

$$F_{01}[\Phi(x+X,t),\Phi_x(x+X,t)] = \frac{\partial F(\phi_c,\phi_c')}{\partial\phi_c'} + \chi'(x,t)\frac{\partial^2 F(\phi_c,\phi_c')}{\partial^2\phi_c'^2} + \chi(x,t)\frac{\partial^2 F(\phi_c,\phi_c')}{\partial\phi_c'\partial\phi_c} \tag{3.4.2}$$

where for notational convenience we have introduced

$$\chi(x,t) = \psi(x,t) + \psi_0(x+X,t)\ . \tag{3.4.3}$$

Substituting Eqs. (3.4.1) and (3.4.2) into Eq. (3.3.24) we have, after collecting terms

$$M_0\ddot{X} = \frac{1}{(1+\xi/M_0)}\Big\{-\int v(x+X,t)\Big[\frac{d}{dx}F(\phi_c,\phi_c')$$

$$
\begin{aligned}
&+ \quad \chi(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c} + \chi'(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c'}\Big] \\
&+ \quad \int (\ddot{\psi}_0(x,t) - \psi_0''(x,t))\phi_c'(x-X)) + \int \phi_c'(x-X)U'[\Phi(x,t)] \\
&+ \quad (1-\dot{X}^2)\int \psi'\phi_c'' - 2\dot{X}\int \dot{\psi}'\phi_c'\Big\} \ . \qquad (3.4.4)
\end{aligned}
$$

Next we write the following Taylor series for $U'[\Phi(x+X,t)]$

$$
U'[\Phi(x+X,t)] = U'[\phi_c(x,t)] + \frac{1}{2}\chi(x,t)U''[\phi_c(x,t)] + \chi^2(x,t)U'''[\phi_c(x,t)] \ , \quad (3.4.5)
$$

where we have used our freedom to choose a normalization such that the following are true

$$
U'[\phi_0] = 0 \quad , \quad U''[\phi_0] = 1 \ , \qquad (3.4.6)
$$

where the potential U has its minimum at ϕ_0. Combining all these terms we have

$$
\begin{aligned}
M_0\ddot{X} &= -\Big(1 - \frac{\xi}{M_0}\Big)\Big[\frac{\partial V(X,t)}{\partial X} + 2\dot{X}\int \dot{\psi}'\phi_c' + \dot{X}^2\int \psi\phi_c''\Big] \\
&- \quad \int v(x+X,t)\Big[\chi(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c} + \chi'(x,t)\frac{d}{dx}\frac{\partial F(\phi_c,\phi_c')}{\partial \phi_c'}\Big] \\
&+ \quad \frac{1}{2}\int \chi^2(x,t)U'''[\phi_c(x)]\phi_c'(x) \ , \qquad (3.4.7)
\end{aligned}
$$

where the effective potential $V(x,t)$ is defined by

$$
V(X,t) = -\int \Big[v(x+X,t)F(\phi_c,\phi_c') - \ddot{\psi}_0(x,t)\phi_c'(x-X)\Big] \ . \qquad (3.4.8)
$$

Equation (3.4.7) is valid through second order in λ. Keeping only the first order terms in λ we have

$$
M_0\ddot{X} = -\frac{\partial V(X,t)}{\partial X} - 2\dot{X}\int \dot{\psi}'\phi_c' - \dot{X}^2\int \psi\phi_c'' \ . \qquad (3.4.9)
$$

Although in principle one must know the phonon field ψ to lowest order in λ before Eq. (3.4.9) can be solved, in practice the terms which involve the phonon field are often small relative to the gradiant of the potential. In order to estimate the magnitude of the phonon field, one must solve the first-order PDE for ψ which is derived below. This in turn requires knowledge of the first-order kink motion. Therefore in principle one must solve a set of coupled equations self-consistently. To make progress without solving the coupled equations, one *assumes* that the ψ field is small. This allows one to solve for the first-order kink motion

$$
M_0\ddot{X} = -\frac{\partial V(X,t)}{\partial X} \ . \qquad (3.4.10)
$$

Given $X(t)$ to lowest order one proceeds to solve the equation for the phonon field (see below). Now one is in a position to check if the gradient term does indeed dominant in Eq. (3.4.9). If this is the case, one may continue to higher order. When the gradient and "phonon" terms are of the same order of magnitude, one must solve the coupled equations self-consistently. This will be the case when the size of the perturbation, that is λ, is much smaller than the initial velocity of the kink. An alternate method involves making a perturbation expansion in both the strength of the perturbation and the initial kink velocity.

A second-order PDE for ψ, valid to first order in the perturbation expansion is derived in Appendix A and is given by

$$\begin{aligned}\ddot{\psi}(x,t) - \psi''(x,t) &+ \psi(x,t)U''(\phi_c) = (1-\mathcal{P}_{\phi_c})\Big\{\Big[1-U''(\phi_c)\Big]\psi_0(x+X,t) \\ &+ v(x+X,t)\Big[F_{10}[\phi_c,\phi_c'] - F_{10}[0,0]\Big] \\ &- \frac{d}{dx}\Big[v(x+X,t)\Big(F_{01}[\phi_c,\phi_c'] - F_{01}[0,0]\Big)\Big]\Big\} \ . \end{aligned} \tag{3.4.11}$$

Since the left-hand side of Eq. (3.4.11) is exactly the small oscillations operator of Eq. (3.1.6), we can write the a solution for $\psi(x,t)$ is terms of a Green function

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt' G(x,x',t-t')I(x',t') \ , \tag{3.4.12}$$

where

$$\begin{aligned} G(x,x',\tau) &= \sum_{i=1}^{N} f_{b,i}^*(x) f_{b,i}(x') \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_{b,i}^2-\omega^2)} \\ &+ \int_{-\infty}^{\infty} f_k^*(x) f_k(x') \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_k^2-\omega^2)} \ , \end{aligned} \tag{3.4.13}$$

with $\tau = t - t'$ and $I(x,t)$ is the right-hand side of Eq. (3.4.11). The Green function in Eq. (3.4.13) contains all of the bound states including the translation mode. At first this seems to contradict the constraint condition in Eq. (3.3.6) because including the translation mode $f_{b,1}(x)$ in the Green function means that $\psi(x,t)$ could have a portion proportional to the translation mode, namely

$$\psi(x,t) = -f_{b,1}^*(x) \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt' f_{b,1}(x') I(x',t') \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_k^2-\omega^2)} \ . \tag{3.4.14}$$

However this is not the case because the expression $I(x',t')$ is manifestly orthogonal to the translation mode and therefore we will find no coefficient of the translation mode. Analytic expressions for the Green function defined in Eq. (3.4.13) in terms of modified Lommel functions of two variables are derived in Chapter 4 for the sine-Gordon, Phi-4 and Double Quadratic potentials [87].

Although one can in principle calculate the ψ field using the Green function, one finds in many cases that it is more cost effective to solve the partial differential equation (3.4.11) directly. One might question the utility of the present perturbation theory if one must, in the end, numerically solve a PDE for ψ when numerical integration of Eq. (3.1.2) solves the entire problem. From a purely computational point of view we could argue that Eq. (3.1.2), unlike Eq. (3.4.11), is a strongly nonlinear PDE and therefore, although there are subroutine packages available which can handle these equations [88], they are often quite costly. Furthermore, although Eq. (3.4.1) may be cumbersome to use in practice, it can be used to deduce general features of the ψ field. For example, consider the situation in which a kink is incident upon a time-independent localized perturbation and scatters to $X = \pm\infty$ (see §5.3). In this case, ψ_0 is time independent and the only time dependence which enters the terms $\psi_0(x + X, t)$ and $v(x + X, t)$ occurring in $I(x, t)$ is through $X(t)$. If the kink scatters to $X = \pm\infty$, for large times $X(t)$ will vary as $V_0 t$ to first order. Since $v(x)$ is localized, both v and ψ_0 will be localized in their first argument. Therefore for large values of t, $\psi_0(x' + X(t'))$ and $v(x' + X(t'))$ will contribute to the integral in Eq. (3.4.1) only for small values of t'. Using the fact that the asymptotic time dependence for the Green function is (see §4.2)

$$G(x, x', t - t') \approx \frac{1}{\sqrt{t - t'}} \ , \tag{3.4.15}$$

one can write

$$\psi(x, t) \approx \int_{-\infty}^{\infty} dx' \int_{t}^{\infty} dt' \frac{I(x', t')}{\sqrt{t - t'}} \ , \tag{3.4.16}$$

$$\approx \frac{1}{\sqrt{t}} \int_{-\infty}^{\infty} dx' \int_{t}^{\infty} dt' \frac{I(x', t')}{\sqrt{1 - t'/t}} \ . \tag{3.4.17}$$

Therefore for fixed x, the ψ field tends to zero for large times, that is to say, there are no long-lived extended phonons generated to this order in the perturbation theory. Similar results have been obtained by Wada and Schriefer [67] and Ogata and Wada [68] when they consider the scattering of a phonon packet (analogous to our ψ_0 field) with a kink. They find that the kink only undergoes a phase shift to lowest order and that no new phonons are emitted. The major difference between their work and ours is that we have a force which maintains the "phonon" packet's shape, however it appears that the effect of this force makes itself felt only in higher order.

Although this result is itself interesting, it has larger implications for the second-order kink motion. Consider the time-dependent second-order terms on the right hand side of Eq. (3.4.7). All of these terms involve either $\psi(x,t)$, which goes to zero as $t \to \infty$, or $\psi_0(x+X(t),t)$. For the scattering situation considered here, $X(t) \to \infty$ as $t \to \infty$; therefore due to the assumed localized nature of the perturbation, $\psi_0(x+X(t),t)$ also goes to zero for large times. Since we already know that the effective potential is zero for large X, the force on the kink for large times is zero. Therefore after the kink has interacted with the perturbation it travels at constant velocity. If some energy has been given to the phonon field this velocity should be less than the initial kink velocity.

The question of the final kink velocity may be attacked more generally by obtaining an approximate first integral of Eq. (3.4.7). To this end we note that given the background field ψ_0, the phonon field ψ, and the first order solution to the kink center of mass motion (i.e. given $X^{(1)}(t)$), the right hand side of Eq. (3.4.7), excluding the $\dot{X}$ term, can be written as a time dependent force denoted by $F(t)$. Also noting that the coefficient of the $\dot{X}$ term is precisely $2\dot{\xi}$, we write

$$(M_0 + \xi(t))\ddot{X} + 2\dot{\xi}\dot{X} = F(t) \ , \tag{3.4.18}$$

where we have also assumed that the $\dot{X}^2$ term is negligible. Multiplying by the integrating factor $(1+\xi/M_0)$ Eq. (3.4.18) may be rewritten as

$$\frac{d}{dt}\Big[M_0(1+\xi/M_0)^2\dot{X}\Big] = (1+\xi/M_0)F(t) \ . \tag{3.4.19}$$

Integrating this equation from $t=-\infty$ to $t=\infty$ we obtain

$$\Big(1+\frac{\xi(\infty)}{M_0}\Big)\dot{X}(\infty) - \Big(1+\frac{\xi(-\infty)}{M_0}\Big)\dot{X}(-\infty) = \frac{1}{M_0}\int_{-\infty}^{\infty} dt' \Big(1+\frac{\xi(t')}{M_0}\Big)F(t') \ . \tag{3.4.20}$$

For the special case in which the perturbation is localized, $\xi(\pm\infty)=0$ which allows us to reduce Eq. (3.4.20) to

$$\dot{X}(\infty) - \dot{X}(-\infty) = \frac{1}{M_0}\int_{-\infty}^{\infty} dt' \Big(1+\frac{\xi(t')}{M_0}\Big)F(t') \ . \tag{3.4.21}$$

These forms allow one to deduce the final kink velocity by performing one numerical integral (this is a very recent result and has not yet been implemented). The expression for the final velocity given in Eq. (3.4.20) should prove to be a good check on the numerical integation of Eq. (3.4.7).

Chapter 4

Nonlinear Klein-Gordon Green Functions

We conclude the formal derivation of the perturbation theory by calculating the Green functions needed to compute the phonon field ψ for the sine-Gordon, ϕ^4 and double quadratic potentials. Recall from section 3.4 that ψ may be expressed as

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt' G(x',x',t-t') I(x',t') \ ,$$

where $I(x',t')$ is an inhomogeneous term which depends on the perturbation. Although this expression for ψ is easy enough to write down, one must ask whether or not it is useful in practice. As mentioned in section 3.4, for the perturbations considered so far we have found that performing the integrals in Eq. (3.4.12) requires too much computation time (I estimate that to compute ψ to 3 significant digits for 1000 values of x and t would require roughly 1 hour of Cray 1 time). This computation requires a lot of time because the Green function oscillates rapidly in t' over the range of times t' for which the inhomogeneous term $I(x',t')$ is appreciable. When one encounters this type of behavior one immediately considers transforming to Fourier space where the Green functions would decay rapidly. This does not help in our case because we have imposed retarded boundary conditions on the Green functions which evidence themselves by the appearance of the step function prefactor $\theta(t-t')$. Next one considers the use of the Laplace transform. When one sees the rather complex analytic form the Green functions take it appears at first that this approach is not possible. It is indeed remarkable that we can obtain analytic forms for the Laplace transform of the Green functions (see section 4.3); however, one is then faced with the nontrivial task of numerically evaluating the Bromwich integral. Although these methods have not yet proved to be useful, it is quite possible that for special perturbations they could lead to analytic expressions for the phonon field.

In the following we derive the Green functions for the sine-Gordon, ϕ^4 and double quadratic nonlinear potentials. One might ask whether other nonlinear potentials could be examined with similar techniques. Since the sine-Gordon and ϕ^4 potentials are the first two of an infinite sequence of nonlinear potentials [49] it is conceivable that this sequence of potentials would be tractable. However, since the phonon waveforms are known analytically [49], we can see that the amount of work needed for each successive potential in the sequence increases linearly, so that one would need to develop a method which applied to the general potential. In addition, it might be desirable to apply different boundary conditions such as periodic boundary conditions on the finite line. However for now we content ourselves with the retarded conditions as applied to the potentials mentioned above.

4.1 Analytic Evaluation of the Green functions

For the set $\{f_{b,i}(x), f_k(x)\}$ of solutions satisfying the "phonon" equation (3.1.8), we define the full Green function as:

$$
\begin{aligned}
G(x,x',\tau) &= \sum_{bound\ states} f^*_{b,i}(x) f_{b,i}(x') \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_i^2-\omega^2)} \\
&+ \int_{-\infty}^{\infty} dk\ f^*_k(x) f_k(x') \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega\tau}}{2\pi(\omega_k^2-\omega^2)} \ , \qquad (4.1.1)
\end{aligned}
$$

where $\tau \equiv t - t'$. Using the completeness relation (3.1.12), and the fact that the set $\{f_{b,i}(x), f_k(x)\}$ satisify equation (3.1.8), one can show that the full Green function satisfies the usual equation:

$$\{\partial_{tt} - \partial_{xx} + U''[\phi_k(x)]\} G(x,x',\tau) = \delta(x-x')\delta(\tau) \ . \qquad (4.1.2)$$

Once a set of boundary conditions is chosen the ω integral in (4.1.1) may be evaluated without choosing a particular set of $\{f_{b,i}(x), f_k(x)\}$. In this paper we choose retarded boundary conditions obtained by moving both of the poles in the ω integral above the real ω axis. Carrying out the ω integral yields:

$$G(x,x',\tau) = G_b(x,x',\tau) + G_p(x,x',\tau) \ , \qquad (4.1.3)$$

where $G_b(x,x',\tau)$ and $G_p(x,x',\tau)$ are the bound state and phonon contributions given by:

$$
\begin{aligned}
G_b(x,x',\tau) &= \theta(\tau)\left\{\tau f^*_{b,1}(x) f_{b,1}(x') + \sum_{i=2}^{N} f^*_{b,i}(x) f_{b,i}(x') \frac{\sin(\omega_i\tau)}{\omega_i}\right\} \ , \qquad (4.1.4) \\
G_p(x,x',\tau) &= \theta(\tau) \int_{-\infty}^{\infty} dk f^*_k(x) f_k(x') \frac{\sin(\omega_k\tau)}{\omega_k} \ , \qquad (4.1.5)
\end{aligned}
$$

with N the number of bound states [if N=1 the second term is omitted from Eq. (4.1.4)] and $\theta(\tau)$ is the Heaviside step function,

$$\theta(\tau) = \begin{cases} 0, & -\infty < \tau < 0 \\ 1 & 0 \leq \tau < \infty \end{cases} \tag{4.1.6}$$

In order to obtain explicit forms for these contributions to the Green function, one must insert the appropriate set of linearized solutions into Eqs. (4.1.4) and (4.1.5). As examples, we evaluate the phonon contribution for the SG, ϕ^4 and DQ potentials.

4.1.1 The sine-Gordon Potential

Since the bound state contribution (4.1.4) is already expressed in terms of known functions, we turn to the evaluation of the phonon contribution given in Eq. (4.1.5). Inserting the functions $f(x)$ from the SG column of Table 3.1 into Eq. (4.1.5) we have, after collecting common terms,

$$G_p^{SG}(x, x', \tau) = \theta(\tau)\{I_1 + \beta_2 I_2 + \beta_3 sgn(z) I_3\} \ , \tag{4.1.7}$$

where

$$\begin{aligned} I_1 &= \frac{1}{\pi}\int_0^\infty \frac{dk}{\sqrt{1+k^2}} \cos(|z|k)\sin(\tau\sqrt{1+k^2}) \ , \\ I_2 &= \frac{1}{\pi}\int_0^\infty \frac{dk}{(1+k^2)^{\frac{3}{2}}} \cos(|z|k)\sin(\tau\sqrt{1+k^2}) \ , \\ I_3 &= \frac{1}{\pi}\int_0^\infty \frac{dk}{(1+k^2)^{\frac{3}{2}}} k\sin(|z|k)\sin(\tau\sqrt{1+k^2}) \ , \end{aligned} \tag{4.1.8}$$

with the definitions

$$\tau \equiv t - t' \quad , z \equiv x - x', \quad \beta_2 \equiv \tanh(x)\tanh(x') - 1, \quad \beta_3 \equiv \tanh(x') - \tanh(x) \ . \tag{4.1.9}$$

Since I_2 is uniformly convergent for all $|z|$ and τ, we may differentiate with respect to $|z|$ to obtain

$$I_3 = -\frac{dI_2}{d|z|} \ . \tag{4.1.10}$$

Therefore only $I_1$and I_2 need to be evaluated. These integrals may be evaluated by considering the integral $I(\mu)$ given by

$$I(\mu) = \frac{1}{\pi}\int_0^\infty \frac{dk}{\sqrt{\mu^2+k^2}} \cos(|z|k)\sin(\tau\sqrt{\mu^2+k^2}) \ , \tag{4.1.11}$$

$$= \frac{\theta(\tau-|z|)}{2} J_0(\mu\sqrt{\tau^2-z^2}) \ , \tag{4.1.12}$$

where the integral is found in the tables [89]. The special case $I(1)$, is precisely the integral I_1. Since the derivative of the integrand of Eq. (4.1.11) is a continuous function of both μ and k we may differentiate $I(\mu)$ with respect to μ to obtain

$$I_2 = \lim_{\mu \to 1}\left\{-\frac{dI(\mu)}{d\mu} + \frac{\tau}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{\mu^2+k^2}\cos(|z|k)\cos(\tau\sqrt{\mu^2+k^2})\right\}\ , \tag{4.1.13}$$

$$= \frac{\theta(\tau-|z|)}{2}\sqrt{\tau^2-z^2}J_1(\sqrt{\tau^2-z^2}) + \frac{\tau}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{1+k^2}\cos(|z|k)\cos(\tau\sqrt{1+k^2})\ . \tag{4.1.14}$$

In the integral remaining in (4.1.14) we substitute $k = \sinh(u)$, which gives us

$$\frac{\tau}{2\pi}\int_{-\infty}^{\infty}\frac{dk}{1+k^2}\cos(|z|k)\cos(\tau\sqrt{1+k^2}) \tag{4.1.15}$$

$$= \frac{\tau}{2\pi}\int_{-\infty}^{\infty}\frac{du}{\cosh(u)}\cos[|z|\sinh(u)]\cos[\cosh\tau(u)]\ , \tag{4.1.16}$$

$$= \frac{\tau}{4\pi}\int_{-\infty}^{\infty}\frac{du}{\cosh(u)}\Big\{\cos[|z|\sinh(u)+\tau\cosh(u)] + \cos[\tau\cosh(u)-|z|\sinh(u)]\Big\}\ , \tag{4.1.17}$$

$$= \frac{\tau}{2\pi}\int_{-\infty}^{\infty}\frac{du e^u}{e^{2u}+1}\Big\{\cos[ae^u+be^{-u}]+\cos[ae^{-u}+be^u]\Big\}\ , \tag{4.1.18}$$

$$= \frac{\tau}{2\pi}\int_{0}^{\infty}\frac{dt}{t^2+1}\Big\{\cos[at+\frac{b}{t}]+\cos[\frac{a}{t}+bt]\Big\}\ , \tag{4.1.19}$$

$$= \frac{\tau}{\pi}\int_{0}^{\infty}\frac{dt}{t^2+1}\cos[at+\frac{b}{t}]\ , \tag{4.1.20}$$

where in passing from (4.1.19) to (4.1.20) we have let $t \to 1/t$ in the second cosine term and have defined

$$a \equiv \frac{\tau+|z|}{2}\ , \tag{4.1.21}$$

$$b \equiv \frac{\tau-|z|}{2}\ . \tag{4.1.22}$$

For $b < 0$ the integral in (4.1.20) is found in the tables [90] to be

$$\frac{1}{\pi}\int_{0}^{\infty}\frac{dt}{t^2+1}\cos\Big[at-\frac{|b|}{t}\Big] = \frac{1}{2}e^{(a-b)}. \tag{4.1.23}$$

For $b > 0$ the integral in Eq. (4.1.20) may be expressed in terms of "modified" Lommel functions of two variables [91]. The "modified" functions, namely Lommel functions in which the first argument is pure imaginary, have not been found in the literature. Hence we introduce the notation $\Lambda_n(w,s)$ and $\Xi_n(w,s)$ for the modified functions and give their series representations in terms of Bessel functions:

$$\Lambda_n(w,s) \equiv i^{-n}U_n(iw,s) = \sum_{m=0}^{\infty}\Big(\frac{w}{s}\Big)^{2m+n}J_{2m+n}(s) \ , \qquad (4.1.24)$$

$$\Xi_n(w,s) \equiv i^{-n}V_n(iw,s) = \sum_{m=0}^{\infty}\Big(\frac{w}{s}\Big)^{-2m-n}J_{-2m-n}(s) \ , \qquad (4.1.25)$$

With these definitions, we write for $b > 0$

$$\frac{1}{\pi}\int_0^{\infty}\frac{dt}{t^2+1}\cos[at+\frac{|b|}{t}] = \frac{1}{2}e^{-(a-b)} - \Lambda_1(w,s) \ , \qquad (4.1.26)$$

where

$$s \equiv \sqrt{\tau^2 - z^2} \ , \qquad (4.1.27)$$

$$w \equiv \tau - |z| \ . \qquad (4.1.28)$$

Combining (4.1.23) and (4.1.26) we have for I_2 :

$$I_2 = \frac{1}{2}\tau e^{-|z|} + \theta(\tau - |z|)\Big\{\frac{sJ_1(s)}{2} - \tau\Lambda_1(w,s)\Big\} \ , \qquad (4.1.29)$$

Using Eq. (D.14) from Appendix D we differentiate (4.1.29) with respect to $|z|$ which results in

$$\frac{dI_2}{d|z|} = -\frac{1}{2}\tau e^{-|z|} + \frac{\theta(\tau-|z|)}{2}\Big\{-(\tau+|z|)J_0(s) + 2\tau\Lambda_0(w,s)\Big\} \ . \qquad (4.1.30)$$

In Eqs. (4.1.29) and (4.1.30), I_2 and its derivative appear to have a term which grows linearly in τ, but this is impossible in view of the integral representations of Eqs. (4.1.8). Using asymptotic expressions for the modified Lommel functions, we shall show in section 4.2 that the large τ dependence is actually an inverse square root.

Writing the phonon contribution as

$$G_p^{SG}(x,x',\tau) = \theta(\tau)\Big\{I_1 + \beta_2 I_2 - \beta_3 sgn(z)\frac{dI_2}{d|z|}\Big\} \ , \qquad (4.1.31)$$

we notice that with I_1, I_2 and $\frac{dI_2}{d|z|}$ given by Eqs. (4.1.12), (4.1.29) and (4.1.30), there is a term which does not vanish outside of the "light-cone" (i.e. a term which does not have $\theta(\tau - |z|)$ as a prefactor), namely

$$\theta(\tau)\frac{\tau e^{-|z|}}{2}\Big\{\beta_2 + sgn(z)\beta_3\Big\} \ . \qquad (4.1.32)$$

One can show that this term may be rewritten as

$$-\theta(\tau)\tau f^*_{b,1}(x) f_{b,1}(x'). \tag{4.1.33}$$

Hence, when the bound state contribution is added to Eq. (4.1.31) to obtain the full Green function, we are left with an expression which vanishes identically outside of the light-cone:

$$\begin{aligned} G^{SG}(x,x',\tau) &= \frac{\theta(\tau-|z|)}{2}\Big\{J_0(s)+\beta_2[sJ_1(s)-2\tau\Lambda_1(w,s)] \\ &- \beta_3 sgn(z)[-(\tau+|z|)J_0(s)+2\tau\Lambda_0(w,s)]\Big\} , \end{aligned} \tag{4.1.34}$$

explicitly demonstrating the retarded boundary conditions applied.

4.1.2 The ϕ^4 Potential

With a slight generalization, the techniques used to evaluate the SG Green function may be applied to the ϕ^4 potential. Proceeding along the same lines, we write the phonon contribution as:

$$G_p^{\phi^4}(x,x',\tau) = \frac{\theta(\tau)}{4}\Big\{\gamma_0 I_0 - \gamma_1 sgn(z)\frac{dI_0}{d|z|} + \gamma_2 I_2 + \gamma_3 sgn(z)\frac{dI_2}{d|z|} + I_4\Big\} , \tag{4.1.35}$$

where I_2 and $\frac{dI_2}{d|z|}$ are given in Eqs. (4.1.29-30) and

$$I_0 = \frac{1}{\pi}\int_0^\infty dk \frac{\cos(|z|k)\sin(\tau\sqrt{1+k^2})}{(1+k^2)^{\frac{3}{2}}(1+4k^2)} , \tag{4.1.36}$$

$$\begin{aligned} I_4 &= \frac{1}{\pi}\int_0^\infty dk \frac{(1+4k^2)\cos(|z|k)\sin(\tau\sqrt{1+k^2})}{(1+k^2)^{\frac{3}{2}}} , &(4.1.37)\\ &= 2\theta(\tau-|z|)J_0(s) - 3I_2 , &(4.1.38) \end{aligned}$$

$$\begin{aligned} \gamma_0 &\equiv 9\{\tanh^2(y)\tanh^2(y') - \tanh(y)\tanh(y')\} , \\ \gamma_1 &\equiv 18\{\tanh(y)\tanh^2(y') - \tanh^2(y)\tanh(y')\} , \\ \gamma_2 &\equiv 9\tanh(y)\tanh(y') - 3\tanh^2(y) - 3\tanh^2(y') , \\ \gamma_3 &\equiv 6\tanh(y) - 6\tanh(y') , &(4.1.39)\\ y &\equiv \frac{x}{2} \quad , \quad y' \equiv \frac{x'}{2} , &(4.1.40) \end{aligned}$$

where Eq. (4.1.12) has been used to simplify Eq. (4.1.37). The remaining integral, I_0, may be reduced by partial fractions to

$$I_0 = \frac{4}{3\pi}\int_0^\infty dk \frac{\cos(|z|k)\sin(\tau\sqrt{1+k^2})}{\sqrt{1+k^2}\,(1+4k^2)} - \frac{I_2}{3} , \tag{4.1.41}$$

$$= \frac{4}{3} I_{01} - \frac{1}{3} I_2 \ , \tag{4.1.42}$$

with I_{01} defined by

$$I_{01} = \frac{1}{\pi} \int_0^\infty dk \frac{\cos(|z|k) \sin(\tau\sqrt{1+k^2})}{\sqrt{1+k^2}\ (1+4k^2)} \ . \tag{4.1.43}$$

To evaluate I_{01} we again substitute $k = \sinh(u)$ which gives us

$$I_{01} = \frac{1}{\pi} \int_0^\infty du \frac{\cos[|z| \sinh(u)] \sin[\tau \cosh(u)]}{1 + 4\sinh^2(u)} \ , \tag{4.1.44}$$

$$= \frac{1}{2\pi} \int_0^\infty \frac{tdt}{t^4 - t^2 + 1} \sin\Big[at + \frac{b}{t}\Big] \ , \tag{4.1.45}$$

where in going from Eq. (4.1.43) to (4.1.44) substitutions similar to those made in Eqs. (4.1.15-20) have been made. Factoring the denominator of Eq. (4.1.45), we define

$$\beta_\pm^2 = -\ t_\pm^2 = -\beta_\mp = \frac{-1 \mp i\sqrt{3}}{2} \ , \tag{4.1.46}$$

where $t_\pm^2$ are the roots of $t^4 - t^2 + 1$. Using partial fractions, we may write Eq. (4.1.44) as

$$I_{01} = \frac{1}{2\pi i\sqrt{3}} \Big\{ \int_0^\infty \frac{tdt}{t^2 + \beta_+^2} \sin\Big[at + \frac{b}{t}\Big] - \int_0^\infty \frac{tdt}{t^2 + \beta_-^2} \sin\Big[at + \frac{b}{t}\Big] \Big\} \ , \tag{4.1.47}$$

$$= \frac{-1}{2i\sqrt{3}} [J(\beta_-^2) - J^*(\beta_-^2)] \ , \tag{4.1.48}$$

$$= \frac{-1}{\sqrt{3}} \Im[J(\beta_-^2)] \ , \tag{4.1.49}$$

where $\Im$ denotes the imaginary part and

$$J(\beta^2) = -\ \frac{1}{\pi} \int_0^\infty \frac{tdt}{t^2 + \beta^2} \sin\Big[at + \frac{b}{t}\Big] \ . \tag{4.1.50}$$

The integral defined in Eq. (4.1.49) is a slight generalization of Hardy's integrals for Lommel functions [91, 92]. The evaluation of $J(\beta^2)$ follows Hardy's with a few modifications and is presented in Appendix C for completeness. From Eq. (C.21) in Appendix C we have

$$J(\beta_-^2) = \frac{1}{2} e^{-(a\beta_- - \frac{b}{\beta_-})} - \theta(b) \Lambda_2 \Big[\frac{2b}{\beta_-}, 2\sqrt{ab}\Big] \ , \tag{4.1.51}$$

$$= \frac{1}{2} e^{-\frac{1}{2}(|z|+i\sqrt{3}\tau)} - \theta(\tau - |z|)\Lambda_2(\beta_+ w, s) \ . \tag{4.1.52}$$

Therefore we have for I_{01} :

$$I_{01} = \frac{1}{2\sqrt{3}} e^{-\frac{|z|}{2}} \sin(\omega_2 \tau) + \frac{\theta(\tau - |z|)}{\sqrt{3}} \Im[\Lambda_0(\beta_+ w, s)] \ , \tag{4.1.53}$$

where

$$\omega_2 \equiv \frac{\sqrt{3}}{2} \ , \tag{4.1.54}$$

and we have used

$$\Im[\Lambda_2(\beta_+ w, s)] = \Im[\Lambda_0(\beta_+ w, s) + J_0(s)] = \Im[\Lambda_0(\beta_+ w, s)] \ . \tag{4.1.55}$$

From Eq. (4.1.35) we see that we need a derivative of I_0, and hence I_{01}, with respect to $|z|$. Using Eq. (D.14) and Eqs. (D.26) from Appendix D we have

$$\frac{dI_{01}}{d|z|} = \frac{-1}{4\sqrt{3}} e^{-\frac{|z|}{2}} \sin(\omega_2 \tau) - \frac{\theta(\tau - |z|)}{2\sqrt{3}} \Im[\Lambda_1(\beta_+ w, s)] \ , \tag{4.1.56}$$

where

$$\frac{\beta_+^2 + 1}{\beta_+} = 1 \ , \tag{4.1.57}$$

has also been used. Collecting all of the pieces, we write for the phonon contribution:

$$\begin{aligned} G_p^{\phi^4}(x, x', \tau) &= \frac{\theta(\tau)}{4} \Big\{ \frac{4}{3}\gamma_0 I_{01} - \frac{4}{3}\gamma_1 sgn(z) \frac{dI_{01}}{d|z|} + [\gamma_2 - \frac{\gamma_0}{3} - 3] I_2 \\ &+ sgn(z)[\frac{\gamma_1}{3} + \gamma_3] \frac{dI_2}{d|z|} + 2\theta(\tau - |z|) J_0(s) \Big\}. \end{aligned} \tag{4.1.58}$$

As in the sine-Gordon case one may show that when we combine the "non-retarded" pieces of the phonon contribution, we get exactly the negative of the bound state contribution; specifically we have

$$\frac{1}{8}[\gamma_2 - \frac{\gamma_0}{3} - 3]\tau e^{-\frac{|z|}{2}} - \frac{sgn(z)}{8}[\frac{\gamma_1}{3} + \gamma_3]\tau e^{-\frac{|z|}{2}} = -\tau f_{b,1}^*(x) f_{b,1}(x') \ , \tag{4.1.59}$$

$$\frac{1}{6\sqrt{3}} e^{-\frac{|z|}{2}} \sin(\omega_2 \tau)\gamma_0 + \frac{1}{12\sqrt{3}} e^{-\frac{|z|}{2}} \sin(\omega_2 \tau) sgn(z) \gamma_1 = -\frac{\sin(\omega_2 \tau)}{\omega_2} f_{b,2}^*(x) f_{b,2}(x'). \tag{4.1.60}$$

With the "non-retarded" portion cancelled by the bound state contribution, we have for the full Green function

$$\begin{aligned} G^{\phi^4}(x,x',\tau) &= \theta(\tau-|z|)\Big\{\frac{1}{3\sqrt{3}}\Im[\gamma_0\Lambda_0(\beta_+ w,s)+\frac{1}{2}\gamma_1 sgn(z)\Lambda_1(\beta_+ w,s)] \\ &+ \frac{1}{8}[\gamma_2-\frac{\gamma_0}{3}-3][sJ_1(s)-2\tau\Lambda_1(w,s)] \\ &+ \frac{sgn(z)}{8}[\frac{\gamma_1}{3}+\gamma_3][-(\tau+|z|)J_0(s)+2\tau\Lambda_0(w,s)]+\frac{1}{2}J_0(s)\Big\} \ . \end{aligned} \quad (4.1.61)$$

4.1.3 The Double Quadratic Potential

As a final example, we evaluate the DQ Green function. The phonon contribution in this case is

$$G_p^{DQ}(x,x',\tau) = \frac{\theta(\tau-|z|)}{2}\Big\{I_1-\Big[I_2(z_+)-\frac{dI_2(z_+)}{dz_+}\Big]\Big\} \ , \quad (4.1.62)$$

where I_1 is given in Eq. (4.1.12) [with $\mu = 1$] and $I_2(z_+)$ is given in Eq. (4.1.29) with $|z|$ replaced by $z_+ \equiv |x| + |x'|$. Factoring out the non-retarded piece we have

$$\begin{aligned} G^{DQ}(x,x',\tau) &= \frac{\theta(\tau-|z|)}{2}\Big\{J_0(s)-s_+J_1(s_+)+2\tau\Lambda_1(w_+,s_+) \\ &+ (\tau+z_+)J_0(s_+)+2\tau\Lambda_0(w_+,s_+)\Big\} \ , \end{aligned} \quad (4.1.63)$$

with

$$z_+ \equiv |x| + |x'| \ , \quad (4.1.64)$$

$$w_+ \equiv \tau - z_+ \ , \quad (4.1.65)$$

$$s_+ \equiv \sqrt{\tau^2 - z_+^2} \ . \quad (4.1.66)$$

All three of the Green functions derived above have been checked against numerical integration. Over a large range of values for x, x' and τ, we find agreement to 8 significant digits, which is presently the accuracy of our routines which compute the modified Lommel functions. In addition we have applied the small oscillation operator [see Eq. (4.1.2)] on each of the analytic expressions which, after some tedious algebra, yield the appropriate delta functions. To obtain a final check, we note that by using the orthogonality relation in Eq. (3.1.13) and linear superposition, we see that phonon contribution to the Green functions must be orthogonal to the bound state(s). Numerical integrations confirm this property for all three Green functions.

4.2 Asymptotic Behavior

To obtain asymptotic expressions ($\tau \to \infty$) for the Green functions, we must first find the appropriate limits of the modified Lommel functions. In Appendix E we examine $\Lambda_0(w,s)$ and $\Lambda_1(w,s)$ in the limit as $s \to \infty$ while $w/s \to 1$, which, when w and s are related to τ and z by Eqs. (4.1.27) and (4.1.28), corresponds to $\tau \gg |z|$. This limit is interesting because the expressions for the phonon contributions to the Green functions have a term linear in τ which, in view of the integral expressions, must be cancelled by the other terms.

Since all of the Green functions are expressible in terms of the integrals I_{01}, I_2 and their derivatives with respect to $|z|$ we consider the asymptotic expressions for these quantities first and then combine them to obtain the limits for the Green functions.

To apply the results of Appendix E we must first recast these results in terms of the variables τ and z which are related to w and s by

$$\begin{aligned} w &= \beta(\tau - |z|) \ , \\ s &= \sqrt{\tau^2 - z^2} \ , \end{aligned} \tag{4.2.1}$$

where β is either unity or β_+. From Eqs. (E.31) and (E.32) of Appendix E, we have for $\beta = 1$,

$$\begin{aligned} \Lambda_0(w,s) \approx\ & \frac{J_0(s)}{2} + \frac{e^{-|z|}}{2} + \frac{|z|}{2\tau}\sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4})\Big[1+\frac{2R_4(1,\kappa)}{(8s)^2}\Big] \\ & \sin(s-\frac{\pi}{4})\frac{2R_2(1,\kappa)}{8s}\Big\} + O(\tau^{-\frac{9}{2}}) \ , \end{aligned} \tag{4.2.2}$$

$$\begin{aligned} \Lambda_1(w,s) \approx\ & \frac{e^{-|z|}}{2} - \frac{s}{2\tau}\sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4})\Big[\frac{2[R_2(1,\kappa)-2]}{8s} - \frac{40R_4(1,\kappa)}{(8s)^3}\Big] \\ & -\sin(s-\frac{\pi}{4})\Big[1+\frac{2[R_4(1,\kappa)+12R_2(1,\kappa)]}{(8s)^2}\Big]\Big\} + O(\tau^{-\frac{9}{2}}) \ , \end{aligned} \tag{4.2.3}$$

where $\kappa \equiv w/s$, R_2 and R_4 are defined in Eqs. (E.29), (E.30), and we have used

$$\epsilon(1,\kappa) = \frac{|z|}{s} \tag{4.2.4}$$

$$\sigma_1(1,\kappa) = \frac{\tau}{2s} \ , \tag{4.2.5}$$

$$\sigma_2(1,\kappa) = \frac{\tau}{2|z|} \ , \tag{4.2.6}$$

$$\frac{\sigma_1(1,\kappa)}{\sqrt{1+\epsilon^2(1,\kappa)}} \;=\; \frac{1}{2s} \;, \tag{4.2.7}$$

$$\frac{\epsilon(1,\kappa)\sigma_2(1,\kappa)}{1+\epsilon^2(1,\kappa)} \;=\; \frac{s}{2\tau} \;. \tag{4.2.8}$$

Inserting the expression for $\Lambda_1(w,s)$ in Eq. (4.2.3) into Eq. (4.1.29), we see that the linear τ dependence exactly cancels (for large τ and $\tau \gg |z|$, both $\theta(\tau-|z|)$ and $\theta(\tau)$ are unity), leaving us with:

$$\begin{aligned} I_2 \;\approx\; & \frac{sJ_1(s)}{2} + \frac{s}{2}\sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4})\Big[\frac{2[R_2(1,\kappa)-2]}{8s} - \frac{40R_4(1,\kappa)}{(8s)^3}\Big] \\ & -\sin(s-\frac{\pi}{4})\Big[1+\frac{2[R_4(1,\kappa)+12R_2(1,\kappa)]}{(8s)^2}\Big]\Big\} + O(\tau^{-\frac{7}{2}}) \;. \end{aligned} \tag{4.2.9}$$

In Eq. (4.2.9), I_2 now seems to have a $\sqrt{s}$ and therefore $\sqrt{\tau}$ dependence, however this again exactly cancels when $J_1(s)$ is expanded in its asymptotic series resulting in:

$$\begin{aligned} I_2 \;\approx\; & \frac{1}{2}\sqrt{\frac{2}{\pi s}}\Big\{\sin(s-\frac{\pi}{4})\Big[\frac{15-4[R_4(1,\kappa)+12R_2(1,\kappa)]}{16(8s)}\Big] \\ + \;& \cos(s-\frac{\pi}{4})\Big[\frac{2R_2(1,\kappa)-1}{8} + \frac{5[21/16-R_4(1,\kappa)]}{(8s)^2}\Big]\Big\} + O(\tau^{-\frac{7}{2}}) \end{aligned} \tag{4.2.10}$$

Similarly we have

$$\begin{aligned} \frac{dI_2}{d|z|} \;\approx\; & \frac{|z|}{2}\sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4})\Big[\frac{9+4R_2(1,\kappa)}{2(8s)^2}\Big] \\ + \;& \sin(s-\frac{\pi}{4})\Big[\frac{2R_2(1,\kappa)-1}{(8s)}\Big]\Big\} + O(\tau^{-\frac{7}{2}}) \;. \end{aligned} \tag{4.2.11}$$

Next we turn to the I_{01} expression which involves modified Lommel functions evaluated at $\beta_+ w$ and s. With $\beta=\beta_+$, $\epsilon(\beta,\kappa)$, $\sigma_1(\beta,\kappa)$ and $\sigma_2(\beta,\kappa)$ become

$$\epsilon(\beta_+,\kappa) \;=\; \frac{|z|+i\sqrt{3}\tau}{2s} \;, \tag{4.2.12}$$

$$\sigma_1(\beta_+,\kappa) \;=\; \frac{\tau+i\sqrt{3}\;|z|}{4\pi s} \;, \tag{4.2.13}$$

$$\sigma_2(\beta_+,\kappa) \;=\; \frac{\kappa}{2s}\frac{(\tau+i\sqrt{3}|z|)(\tau+|z|)}{|z|+i\sqrt{3}\tau} \;. \tag{4.2.14}$$

Inserting Eqs. (4.2.12-14) into Eqs. (E.31) and (E.32), we have

$$\Lambda_0(\beta_+ w, s) \approx \frac{1}{2}e^{-\frac{|z|}{2}}e^{i\omega_2 t} + \frac{1}{2}\frac{1}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}}\sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4})\big[1+\frac{2R_4(\beta_+,\kappa)}{(8s)^2}\big]$$
$$+ \sin(s-\frac{\pi}{4})\frac{2R_2(\beta_+,\kappa)}{(8s)}\Big\} + O(\tau^{-\frac{7}{2}}) \;, \qquad (4.2.15)$$

$$\Lambda_1(\beta_+ w, s) \approx \frac{1}{2}e^{-\frac{|z|}{2}}e^{-i\omega_2 t} - \frac{1}{2}\frac{1}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}}\sqrt{\frac{2}{\pi s}} \times$$
$$\times \Big\{\cos(s-\frac{\pi}{4})\big[\frac{2[R_2(\beta_+,\kappa)-2]}{(8s)} - 40\frac{R_4(\beta_+,\kappa)}{(8s)^3}\big]$$
$$- \sin(s-\frac{\pi}{4})\big[1+\frac{2[R_4(\beta_+,\kappa)+12R_2(\beta_+,\kappa)]}{(8s)^2}\big]\Big\}$$
$$+O(\tau^{-\frac{9}{2}}) \;, \qquad (4.2.16)$$

where we have used

$$\frac{\sigma_1(\beta_+,\kappa)}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}} = \frac{1}{2} \;, \qquad (4.2.17)$$
$$\frac{\epsilon(\beta_+,\kappa)\sigma_2(\beta_+,\kappa)}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}} = \frac{1}{2} \;, \qquad (4.2.18)$$

When Eq. (4.2.15) is inserted into the expression for I_{01}, the oscillatory term in τ cancels leaving us with

$$I_{01} \approx \frac{1}{2\sqrt{3}}\Im\Big\{\frac{1}{\sqrt{1+\epsilon^2(1,\kappa)}}\sqrt{\frac{2}{\pi s}}\big[\cos(s-\frac{\pi}{4})(1+\frac{2R_4(\beta_+,\kappa))}{(8s)^2})$$
$$+ \sin(s-\frac{\pi}{4})\frac{2R_2(\beta_+,\kappa)}{(8s)}\big]\Big\} + O(\tau^{-\frac{7}{2}}) \;, \qquad (4.2.19)$$

and

$$\frac{dI_2}{d|z|} \approx \frac{1}{2\sqrt{3}}\Im\Big\{\frac{1}{\sqrt{1+\epsilon^2(1,\kappa)}}\sqrt{\frac{2}{\pi s}}\big[\cos(s-\frac{\pi}{4})\big(\frac{2[R_2(\beta_+,\kappa)-2]}{8s}\big)$$
$$- \sin(s-\frac{\pi}{4})\big(1+\frac{2[R_4(\beta_+,\kappa)+12R_2(\beta_+,\kappa)]}{(8s)^2}\big)\big]\Big\} + O(\tau^{-\frac{7}{2}}) \;, \qquad (4.2.20)$$

Now all of the contributions are at hand to obtain, through $O(\tau^{-\frac{7}{2}})$, the asymptotic forms for the Green functions. However, since the expressions are lengthy and not particularly illuminating, we list only the leading terms. Due to the simple analytic form of the bound state contribution, we list only the phonon portions:

$$G_p^{SG}(x,x',\tau) \approx \sqrt{\frac{2}{\pi s}}\Big\{\cos(s-\frac{\pi}{4}) + \frac{1}{8s}\sin(s-\frac{\pi}{4})\Big\} + O(\tau^{-\frac{5}{2}}) \ , \tag{4.2.21}$$

$$\begin{aligned} G_p^{\phi^4}(x,x',\tau) \approx \sqrt{\frac{2}{\pi s}}\Big\{&\cos(s-\frac{\pi}{4})\Big[\frac{\gamma_0}{6\sqrt{3}}\Im\Big(\frac{1}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}}\Big) \\ +\ & \frac{1}{8}\Big(\gamma_2 - \frac{\gamma_0}{3} - 3\Big)\Big(\frac{2R_2(1,\kappa)-1}{8}\Big) + 2\Big] \\ -\ & \sin(s-\frac{\pi}{4})\Big[\frac{\gamma_1 sgn(z)}{12\sqrt{3}}\Im\Big(\frac{1}{\sqrt{1+\epsilon^2(\beta_+,\kappa)}}\Big)\Big]\Big\} + O(\tau^{-\frac{3}{2}}) \ , \end{aligned} \tag{4.2.22}$$

$$G_p^{DQ}(x,x',\tau) \approx \sqrt{\frac{2}{\pi s}}\cos(s-\frac{\pi}{4}) - \frac{1}{2}\sqrt{\frac{2}{\pi s_+}}\cos(s_+-\frac{\pi}{4})\Big[\frac{2R_2(1,\kappa_+)-1}{8}\Big] + O(\tau^{-\frac{3}{2}}) \ , \tag{4.2.23}$$

where in Eq. (4.2.23), $\kappa_+ \equiv w_+/s_+$.

One may notice that although we have shown that there is no linear τ term in the phonon contributions to the Green functions, the full Green functions have a linear τ term due to the first bound state, namely,

$$\theta(\tau)\tau f_{b,i}^*(x) f_{b,i}(x') \ . \tag{4.2.24}$$

This term may be understood by realizing that when computing the response of a soliton to a perturbation, the effect of this term is to produce a coefficient of the translation mode $f_{b,1}(x)$ which increases with time. Therefore, the soliton will move from its initial position as time progresses. Hence in this case, the linear term is required to describe the translation of the soliton.

The secularity referred to in the introduction is made evident by the linear τ behavior in the coefficient of the translation-mode contribution to the full Green function. Indeed, the use of the full Green function in a perturbation theory of kink dynamics in the presence of external influences is equivalent to the procedure introduced by Fogel et al.[37]. The use of the collective-coordinate method avoids the secularity associated with the translation mode since only the "phonon" part of the Green function is employed (together with the contribution from other bound states, if any ($N \geq 2$)).

4.3 Laplace Transform of the SG Green function

As mentioned in the beginning of this chapter, we can obtain analytic forms for the Laplace transform of the Green functions. In the interest of brevity we present only the transformation for the SG Green functions although the methods below also apply to the other models (ϕ^4 and DQ). From Eq. (4.1.34) we see that Laplace transform of the SG Green function is made up of a sum of the Laplace transform of several Bessel functions plus the Laplace transform of the modified Lommel functions. The Bessel function transforms are easily found in the tables [93] or may be written as derivatives of known transforms and therefore we merely present these results. Defining the Laplace transform of a function $F(\tau)$ to be

$$\bar{F}(\bar{s}) = \mathcal{L}[F(\tau)] \equiv \int_0^\infty d\tau e^{-\bar{s}\tau} F(\tau) \ , \tag{4.3.1}$$

we easily obtain the following:

$$\mathcal{L}\Big[\theta(\tau - |z|) J_0(\sqrt{\tau^2 - |z|^2})\Big] = \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\sqrt{\bar{s}^2+1}} \ , \tag{4.3.2}$$

$$\mathcal{L}\Big[\theta(\tau - |z|)\sqrt{\tau^2 - |z|^2} J_1(\sqrt{\tau^2 - |z|^2})\Big] = \left[\frac{1}{\sqrt{\bar{s}^2+1}} + |z|\right] \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\bar{s}^2+1} \tag{4.3.3}$$

$$\mathcal{L}\Big[\tau\theta(\tau - |z|) J_0(\sqrt{\tau^2 - |z|^2})\Big] = \left[\frac{1}{\sqrt{\bar{s}^2+1}} + |z|\right] \frac{\bar{s}}{\sqrt{\bar{s}^2+1}} \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\sqrt{\bar{s}^2+1}} \tag{4.3.4}$$

With these expressions in hand it remains to compute the Laplace transform of the modified Lommel functions.

4.3.1 Laplace Transform of $\theta(\tau - |z|)\Lambda_n(w, s)$

Recalling the definition for the modified Lommel functions of two variables, we write for $\Lambda_n(w, s)$

$$\Lambda_n(w, s) = \sum_{m=0}^\infty \left(\sqrt{\frac{\tau - |z|}{\tau + |z|}}\right)^{n+2m} J_{n+2m}(\sqrt{\tau^2 - |z|^2}) \ . \tag{4.3.5}$$

Since we always have $\tau > |z|$, this sum converges uniformly and therefore in taking the Laplace transform of the sum we can interchange the order of integration and summation. Therefore we are led to consider the Laplace transform of the summand in Eq. (4.3.5) which is found in the tables [94] to be

$$\mathcal{L}\left[\left(\sqrt{\frac{\tau - |z|}{\tau + |z|}}\right)^{n+2m} J_{n+2m}(\sqrt{\tau^2 - |z|^2})\right] = \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\sqrt{\bar{s}^2+1}(\sqrt{\bar{s}^2+1} + \bar{s})^{n+2m}} \ . \tag{4.3.6}$$

Therefore

$$\begin{aligned}
\mathcal{L}[\theta(\tau-|z|)\Lambda_n(w,s)] &= \sum_{m=0}^{\infty}\frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\sqrt{\bar{s}^2+1}}\left[\frac{1}{\sqrt{\bar{s}^2+1}+\bar{s}}\right]^{n+2m} \\
&= \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{\sqrt{\bar{s}^2+1}}\left[\frac{1}{\sqrt{\bar{s}^2+1}+\bar{s}}\right]^{n-2}\frac{1}{2\bar{s}}\frac{1}{\sqrt{\bar{s}^2+1}+\bar{s}} \qquad (4.3.7)
\end{aligned}$$

where in evaluating the sum I have used the fact that when doing an inverse Laplace transform, $\Re(\bar{s}) > 0$ and therefore the sum converges uniformly. Now all of the components are at hand to obtain the expression for the Laplace transform of the SG Green function. In doing the algebra, quite a bit of cancellation occurs leaving us with a remarkably simple expression for the Laplace transform

$$\begin{aligned}
\bar{G}^{SG}(x,x';\bar{s}) &\equiv \mathcal{L}[G(x,x',\tau)] \\
&= \frac{e^{-|z|\sqrt{\bar{s}^2+1}}}{2}\left\{\frac{1}{\sqrt{\bar{s}^2+1}} - \frac{\beta_2}{\bar{s}^2\sqrt{\bar{s}^2+1}} - \frac{\beta_3 sgn(z)}{\bar{s}^2}\right\} . \qquad (4.3.8)
\end{aligned}$$

4.3.2 Bromwich Representation for $\psi(x,t)$

The derivation of the Laplace transform is not merely an academic execise as it may prove useful for the numerical evaluation of the phonon field. To see that this is the case we now substitute the inverse Laplace representation of the SG Green function into the integral expression for ψ given in Eq. (3.4.12)

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt' \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\bar{s}\; e^{\bar{s}\tau}\bar{G}^{SG}(x,x';\bar{s})I(x',t') \qquad (4.3.9) \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dt'\; \bar{G}^{SG}(x,x';c+iy)e^{-(c+iy)(t'-t)}I(x',t') \qquad (4.3.10)
\end{aligned}$$

where c is a positive real constant which is greater than 0 (i.e. this is the real part of the "right-most" pole of $\bar{G}^{SG}(x,x';\bar{s})$). To make further analytic progress, we consider a specific perturbation, namely we choose a linear coupling function $F = \Phi$ and a time-independent perturbation which is well localized in space

$$v(x) = \lambda\left\{e^{-(x-x_0)^2} - e^{-(x+x_0)^2}\right\} , \qquad (4.3.11)$$

(this is one of the perturbations examined in Chapter 5). In this case the inhomogeneous term $I(x',t')$ may be written as

$$I(x',t') = \psi_0(x'+X(t'))\text{sech}^2(x') - \frac{\phi_c'(x')}{M_0}\int_{-\infty}^{\infty} dz\; \phi_c'(z)\psi_0(z+X(t'))sech^2(z) , \qquad (4.3.12)$$

where the “background response” field ψ_0 satisifies

$$-\psi_0'' + \psi_0 = v(x) \ . \tag{4.3.13}$$

We can solve for ψ_0 by Fourier transforming and to this end we introduce the following inverse transforms

$$\bar{\psi}_0(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ e^{ikx} \psi_0(x) \ , \tag{4.3.14}$$

$$\bar{v}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\ e^{ikx} v(x) \ . \tag{4.3.15}$$

By substituting these transforms into Eq. (4.3.13) we see that they are related by

$$\bar{\psi}_0(k) = \frac{\bar{v}(k)}{1+k^2} \ . \tag{4.3.16}$$

Next we consider the t' integral in Eq. (4.3.10)

$$\int_{-\infty}^{\infty} dt' e^{-(c+iy)t'} I(x', t') \ . \tag{4.3.17}$$

From Eq. (4.3.12) we see that the only t' dependence occurs through $X(t')$. To lowest order we approximate this by

$$X(t') \approx X_0 + V_0 t' \ , \tag{4.3.18}$$

where $X_0 \equiv X(0)$ and $V_0 \equiv \dot{X}(0)$. By assuming Eq. (4.3.18) to be valid, we restrict ourselves to the study of the case in which the kink scatters off the perturbation to ∞. We are therefore led to consider the integral

$$J(\xi, y; c) \equiv \int_{-\infty}^{\infty} dt' e^{-(c+iy)t'} \psi_0(\xi + X_0 + V_0 t') \tag{4.3.19}$$

$$= \frac{e^{i(\xi+X_0)(y-ic)/V_0}}{V_0} \int_{-\infty}^{\infty} d\zeta\ e^{-i\zeta(y-ic)/V_0} \psi_0(\zeta) \ , \tag{4.3.20}$$

where ξ is either x' or z as required by Eq. (4.3.12). Although the integrand seems to diverge as $\zeta \to -\infty$ it does not since one can show that for the perturbation chosen we have

$$\bar{v}(k) \approx e^{-k^2} \tag{4.3.21}$$

and therefore

$$\psi_0(x) \approx \int_{-\infty}^{\infty} dk \frac{e^{-k^2} e^{-ikx}}{1+k^2} \ , \tag{4.3.22}$$

and hence $\psi_0(x)$ will decay faster than e^{-x^2}. Since the integral converges we may analytically continue it and obtain the result

$$J(\xi, y; c) = \sqrt{2\pi} \frac{e^{i(\xi+X_0)(y-ic)/V_0}}{V_0} \bar{\psi}_0\Big(\frac{y-ic}{V_0}\Big) \ . \tag{4.3.23}$$

Having carried out the above integration we return to the expression (4.3.12) for $I(x', t')$ and find that this integral occurs inside the spatial integral over z and therefore we consider the integral

$$\frac{\sqrt{2\pi}}{V_0} e^{iX_0(y-ic)/V_0} \bar{\psi}_0\Big(\frac{y-ic}{V_0}\Big) \int_{-\infty}^{\infty} dz \ \phi_c'(z) \mathrm{sech}^2(z) e^{iz(y-ic)/V_0} \ . \tag{4.3.24}$$

Again it seems that this integral

$$\int_{-\infty}^{\infty} dz \ \mathrm{sech}^3(z) e^{iz(y-ic)/V_0} \tag{4.3.25}$$

may not converge due to the factor of e^{zc/v_0} (I have used the fact that $\phi_c'(z) = 2\mathrm{sech}(z)$ for SG). Since c needs only to be > 0, we can choose it such that

$$\frac{c}{V_0} < 3 \tag{4.3.26}$$

so that the $\mathrm{sech}^3(z)$ factor will dominate. Using the fact that the integral does indeed exist, we analytically continue a standard result from the Tables [95] to obtain

$$\int_{-\infty}^{\infty} dz \ \mathrm{sech}^3(z) e^{iz(y-ic)/V_0} = \pi \left[\left(\frac{4-ic}{V_0} \right)^2 + 1 \right] \mathrm{sech}\Big[\frac{\pi(y-ic)}{2V_0}\Big] \ . \tag{4.3.27}$$

Using all of these pieces we can write another integral expression for the phonon field

$$\begin{aligned} \psi(x,t) &= \frac{e^{ct} e^{cX_0/V_0}}{V_0 \sqrt{2\pi}} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy \bar{G}^{SG}(x, x'; c+iy) \frac{e^{iyt}}{\cosh x'} \bar{\psi}_0\Big(\frac{y-ic}{V_0}\Big) \times \\ &\times \left\{ \frac{e^{ix'(y-ic)/V_0}}{\cosh(x')} - \frac{2\pi}{M_0} \Big[\Big(\frac{y-ic}{V_0}\Big)^2 + 1 \Big] \mathrm{sech}\Big[\frac{\pi(y-ic)}{2V_0}\Big] \right\} \ . \end{aligned} \tag{4.3.28}$$

Again we must evaluate a two-dimensional integral to obtain values for ψ, however this integrand has a rapidly decaying factor, namely the Laplace transform of the Green function. However, the exponential factor

$$e^{ix'(y-ic)/V_0} \tag{4.3.29}$$

still oscillates rapidly in y since typical values of X_0 and V_0 are -10 and .3 respectively. In addition we have an exponential term in time which also yields rapid oscillations for large t. However this type of oscillating behavior may prove to be the key to a quick and efficient evaluation of Eq. (4.3.28). The key lies in the fact that the evaluation of Eq. (4.3.28) is written in "Fourier transform form". The fact that the integrand in Eq. (4.3.28) already involves Fourier transform of the ψ_0 field and therefore the possibility of using the convolution theorem exists. If nothing else, we have in Eq. (4.3.28) an approximate analytic expression (in terms of an integral) of the time Fourier transform for the ψ field

Assuming that Fourier transform methods are not tractable, the ease with which Eq. (4.3.28) is evaluated depends on whether the oscillations are damped quickly enough by the decaying factors. In addition to the rapid decay caused by the Laplace transform of the Green function, the Fourier transform of the background field is also rapidly decaying. For the perturbation examined in this section, we have the following analytic form for $\bar{\psi}_0$:

$$\bar{\psi}_0 = \frac{2\sqrt{\pi}\cos kx_0 e^{-k^2/4}}{1+k^2} \ . \tag{4.3.30}$$

With this additional decaying factor, it is quite possible that this integral may be done numerically. One of the major problems with the previous two-dimensional integral expression for the ψ field is that one had to evaluate the Green function itself, which involves calculating and summing approximately 200 Bessel functions. Even when these codes are vectorized and run on a Cray-1 computer, these manipulations require quite a bit of time. In view of the problems encountered with the numerical integration of the ψ PDE (see §5.2), numerical evaluation of ψ using Eq. (4.3.28) is a very attractive possibility which is currently under investigation.

4.4 Representative plots

To illustrate the behavior of the Green functions we present several plots of the *phonon* part of the SG Green function [plots for the other Green functions derived look very similar] . The numerical values for these plots are easily obtained from the formulae in Appendix E.

We can get a feel for how the Green functions should behave by recalling that $G(x, x', t - t')$ represents the response of the field at (x, t) due to a delta function source at (x', t'). To make this more concrete we can imagine striking one of the pendula of the sine-Gordon pendulum chain with a sharp blow and watching the response of the other pendula. We expect to see a pulse move out from the "hit pendulum" and propagate toward the ends of the chain. In Figure 4.1 we plot the Green function vs. x and x' for various values of $t = \tau$ (we have chosen $t' = 0$). Fixing $x' = 8$ (i.e. the pendulum at $x = 8$ is struck) in Figure 4.1a, we move in the direction of increasing x, starting at $x = 0$. Until x is on the order of 2, $G(x, x', \tau)$ is zero, meaning that the disturbance has not yet had enough time to propagate from $x = 8$ to $x < 2$ (or $x > 14$). For $\tau = 4$, time has progressed (recall we have fixed $t' = 0$) and the disturbance has propagated further outwards. At $t = 8$ the pulse reaches $x = 8$. In Figures 4.1e to 4.1h the pulse has propagated off the scales, leaving behind "ripples". As τ further increases the amplitude continues to decrease in accord with the asymptotic behavior derived in section 4.2.

If one were to follow the procedure outlined in the preceding paragraph with $x' = 3$, one would note that before the pulse arrives at a particular position, the Green function is not zero. This is because we have plotted the phonon contribution, which has a non-retarded part which exactly cancels the bound state contribution. It is this non-retarded part which gives a non-zero value for the phonon contribution to the Green function "before the pulse arrives". We see this only near $x = x' = 0$ because the bound state contribution is proportional to $e^{-|z|}$ [SG], $\text{sech}(x)\text{sech}(x')$ [ϕ^4] or $e^{-|x|}e^{-|x'|}$ [DQ].

Since the computation of the phonon response ψ involves integrals of the Green function over x' and t', it is interesting to see the behavior of $G(x, x', t - t')$ for fixed x and t. In Figure 4.2 we plot the sine-Gordon Green function for $x = 25$ and $t = 50$. One of the interesting features is the step function which represents the "light cone". In performing the numerical integrals one must be careful not to integrate through this step function since most numerical integrators cannot handle such discontinuities. Another feature which presents some numerical difficulties is the oscillation in time. Of course this oscillation will represent problems only if we must integrate over several of these periods (which is in fact the case for the perturbations examined in Chapter 5).

In Figure 4.3 we present illustrates one of the asymptotic limits of the Green functions. The fact that the Green functions are not functions solely of $x - x'$ is a consequence of the broken translational invariance which results from the introduction of a kink. The only dependence on x and x' which is not through the combination $x - x'$ enters through the functions β_i (SG) and γ_i (ϕ^4). All of these functions depend on x and x' through various combinations of $\tanh(x)$ and $\tanh(x')$. For both x and x' large these β and γ factors are constants so one expects that for both x and x' large the Green functions should depend only on $x - x'$. This fact is illustrated by the plot in Figure 4.3. One can understand this fact analytically by recalling that the functions $f_k(x)$ which are used to define the

Figure 4.1: The time evolution for the phonon contribution to the SG Green function $G(x, x', t - t')$ in the $x - x'$ plane.

Figure 4.2: The phonon contribution to the SG Green function $G(x, x', t - t')$ in the $x' - t'$ plane.

Figure 4.3: The SG Green function $G(x, x', t - t')$ in the $x - x'$ plane. Note the reflection symmetry about the $x = x'$ line.

Green functions are asymptotically plane waves for large x and hence this behavior is to be expected. This behavior may prove useful for certain perturbations if one must perform integrals only over this translationally invariant region.

Figures 4.4 and 4.5 show plots of the real part of the Laplace transform of the sine-Gordon Green function. In Figure 4.4 we plot the real part of the Laplace transform $\bar{G}^{SG}(x, x', \bar{s})$ vs. x and x' for fixed $\bar{s} = 2+2i$. Here we see the dominance of the exponential factor $e^{-|z|\sqrt{\bar{s}^2+1}}$ in Eq. (4.3.8) since the modulus of $\bar{s}$ is large enough so that the factors which do not depend on $x - x'$, that is the factors involving β_2 and β_3, are small compared with the first term in Eq. (4.3.8). The rapid decay in x' shown in Figure 4.4 makes the integral in Eq. (4.3.28) converge rapidly. One might think that the cusp shown in this figure would pose a problem when Eq. (4.3.28) is numerically evaluated. However, one must realize that the integral in Eq. (4.3.28) is not over the $x - x'$ plane but over the $x' - \bar{s}_i$ plane where $\bar{s}_i$ is the imaginary part of the Laplace transform variable. To get a feel for the dependence on the Laplace transform variable $\bar{s}$, we plot in Figure 4.5 the real part of the Laplace transform $\bar{G}^{SG}(x, x'; \bar{s})$ in the complex $\bar{s}$ plane for $x = 2.0$ and $x' = 1.0$. The interesting feature in this plot is the dependence on the imaginary part of $\bar{s}$ which is a rapid decay. Again this is not surprising since the analytic expression given in Eq. (4.3.8) involves an exponential factor of the form

$$e^{-|z|\sqrt{\bar{s}^2+1}} .$$

Since the Bromwich integral for the ψ field involves integrating in the complex $\bar{s}$ plane along a line parallel to the imaginary $\bar{s}$ axis, this rapid decay should greatly facilitate the numerical calculations.

Figure 4.4: The real part of the Laplace transform of the sine-Gordon Green function $\bar{G}^{SG}(x, x'; \bar{s})$ plotted vs. x and x' for $\bar{s} = 2 + 2i$.

Figure 4.5: The real part of the Laplace transform of the sine-Gordon Green function $\bar{G}^{SG}(x, x'; \bar{s})$ plotted in the complex $\bar{s}$ plane for $x = 2.0$ and $x' = 1.0$.

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

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

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

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

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 $\pm x_0$

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

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

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

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

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

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)

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

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,

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

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

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

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,

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

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

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

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

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

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

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

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

where we have made use of the identity in Eq. (3.1.15). Since $1 - U''(\phi_c(x')) = 2\mathrm{sech}^2(x')$ and $\phi_c'(x) = 2\mathrm{sech}(x')$ (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

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

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.

Chapter 6

Thermal Noise

Since every physical system is subject to thermal fluctuations, it is important to consider the effects of such noise on the motion of kinks. The two standard methods which are employed are the Langevin [107] and Fokker-Planck [107, 108, 109] techniques. Each has its advantages and disadvantages. Although the Langevin approach is somewhat simpler to use, it is an equilibrium calculation and therefore one does not get information about the approach to equilibrium. This is an important question for the soliton bearing systems we are dealing with because we have essentially two quite different degrees of freedom to treat, namely the kink itself and the phonons. It is often assumed that the phonon degrees of freedom are adiabatic, that is, if the system is jarred from equilibrium, it is assumed that the phonon degrees of freedom will equilibrate very quickly about the instantaneous kink position and velocity. Although this seems to be quite a reasonable assumption, one must really confirm this and the Fokker-Planck technique is one way to do this.

In the Fokker-Planck method [108], one writes an equation for the time-dependent, phase-space probability distribution function, $P(X, p; t)$. If the system is not driven, $P(X, p; \infty)$ represents the equilibrium distribution function familiar from classical equilibrium statistical mechanics. In the driven case, $P(X, p; \infty)$ represents the steady-state distribution function. With the full time-dependent function one can compute time-dependent averages such as

$$\langle X(t) \rangle = \int_{-\infty}^{\infty} dX \int_{-\infty}^{\infty} dp \; X \; P(X, p; t) \; .$$

Since one can also compute $\langle X(t) \rangle$ via the Langevin approach, it is not here where the strength of the Fokker-Planck method lies. Rather, one can find the time needed to reach equilibrium. This is done by solving the Fokker-Planck equation for $P(X, p; t)$ with initial conditions which are far from equilibrium such as

$$P(X, p, 0) = \delta(X - X_0)\delta(p - p_0) \; .$$

Although one cannot often find the exact time-dependent solution to the Fokker-Planck equation, the question of the equilibration time can be settled by finding only the lowest nonzero eigenvalue. In addition to the standard methods available for this, there are more modern supersymmetric methods [110] which can also be of great value.

A third and somewhat nonstandard approach has been used by Wada and Schrieffer [67] (WS). They calculate a "diffusion constant" by using the fluctuation-dissipation theorem [67, 111]

$$D = \lim_{t\to\infty} \frac{\langle X^2(t)\rangle}{2t} \ .$$

The calculation needed here is of course $\langle X^2(t)\rangle$. To this end, they begin with a stationary kink and calculate the shift in the kink position ($X(t)$) which results from the collision of a kink with a phonon packet which they assume to be thermally excited according to the distribution function

$$P_{eq}(\psi, \pi) = e^{-\beta H_{ph}} \ ,$$

where $\beta = T^{-1}$ ($k_B = 1$ in our units) and H_{ph} is given by

$$H_{ph} = \int \Big[\frac{1}{2}\pi^2 + \frac{1}{2}\psi'^2 + \frac{1}{2}\psi^2 U''(\phi_c)\Big] \ .$$

Assuming such a distribution function seems to be quite a reasonable choice, however no basis was given for the choice. It also implicitly assumes that the phonons are in equilibrium but the kink is not. In real physical systems this distinction cannot be made. For example, in the sine-Gordon pendulum chain, such thermal fluctuations could be simulated by submerging the entire chain into a viscous medium at some finite temperature. All of the pendula experience a random force, so when a transformation is made to another set of basis functions, it is unreasonable to assume that some of these modes feel the random force while others do not. In disregarding this feature, WS's method yields the unphysical result that the initial velocity of the kink is undamped (see section 6.1), not at all like the Brownian motion one might expect in view of the large body of evidence which indicates that the kink behaves like an extended Newtonian particle. One of the conclusions of this chapter is that we do indeed find that to lowest order the kink behaves like a Brownian particle. We illustrate this by using both the Langevin and Fokker-Planck methods. However, before we consider these techniques, calculations are presented which verify the claim made above with regards to the undamped motion of the kink.

6.1 Thermalized Phonon Ansatz

To demonstrate that the assumptions of WS imply that the initial velocity of a particle is undamped, we explicitly calculate $\langle X^2(t)\rangle$ (through second order) using the equation of motion (3.4.7) derived in Chapter 3. Since WS assume no direct coupling to a heat bath, the perturbation is zero, in which case Eq. (3.4.7) takes on the form

$$\ddot{X}(t) = -\eta_\psi \dot{X}(t) + F_\psi \ , \tag{6.1.1}$$

where we have taken ψ_0 to be zero and introduced the following definitions

$$\eta_\psi \equiv \frac{-2}{M_0}\int dx\ \dot{\psi}(x,t)\phi_c''(x)\ , \tag{6.1.2}$$

$$F_\psi \equiv \frac{1}{2M_0}\int dx\ U'''[\phi_c(x)]\psi^2(x,t)\phi_c'(x)\ . \tag{6.1.3}$$

Above we claim that Eq. (6.1.1) holds through second order. However, since we have no (formal) perturbation, this statement requires clarification. In using WS's approach, the perturbation enters the problem indirectly through the assumption that the phonons are thermally distributed. Therefore the proper expansion parameter for low temperatures is T/M_0 where M_0 is the kink rest energy in our units. Since the phonons are Gaussian-distributed (see below), we can use the equipartition theorem to assign a $\sqrt{T}$ power to the ψ field. In section 6.2 we show that the kink also obeys the equipartition theorem to lowest order and therefore we assign a $\sqrt{T}$ power to $\dot{X}$. Therefore, the right-hand side of Eq. (6.1.1) is correct to order T, that is to second order in $\sqrt{T}$.

WS used Eq. (6.1.1) without the "inertial" term η_ψ, and performed averages over the phonon degrees of freedom by assuming for the equilibrium distribution function for the phonons,

$$P_{eq} = e^{-\beta H_{ph}}\ , \tag{6.1.4}$$

with H_{ph} given by

$$H_{ph} = \int \Big[\frac{1}{2}\pi^2(x,t) + \frac{1}{2}\psi'^2(x,t) + \frac{1}{2}\psi^2(x,t)U''[\phi_c(x)]\Big]\ . \tag{6.1.5}$$

To do the explicit calculations we use the following normal mode representations

$$\psi(x,t) = \sum_k \frac{1}{\sqrt{2\omega_k}}\Big[b_k f_k(x)e^{-i\omega_k t} + b_k^* f_k^*(x)e^{i\omega_k t}\Big]\ , \tag{6.1.6}$$

$$\pi(x,t) = \sum_k -i\sqrt{\frac{\omega_k}{2}}\Big[b_k f_k(x)e^{-i\omega_k t} - b_k^* f_k^*(x)e^{i\omega_k t}\Big]\ , \tag{6.1.7}$$

which allows us to write

$$H_{ph} = \sum \omega_k |b_k|^2 \ . \tag{6.1.8}$$

Using this representation we present the following quantities which have been computed in Appendix F:

$$\langle b_k^* b_{k'} \rangle = \frac{T}{\omega_k} \delta_{k,k'} \ , \tag{6.1.9}$$

$$\langle \psi^2(x,t) \rangle = T \sum_k \frac{|f_k(x)|^2}{\omega_k^2} \ , \tag{6.1.10}$$

where the average denoted by the brackets $\langle\rangle$ is defined by

$$\langle F(b_q, b_{q'}^*) \rangle = \frac{\prod_k \int_{-\infty}^{\infty} db_k \int_{-\infty}^{\infty} db_k^* \ F(b_q, b_{q'}^*) e^{-\beta\omega_k |b_k|^2}}{\prod_k \int_{-\infty}^{\infty} db_k \int_{-\infty}^{\infty} db_k^* \ e^{-\beta\omega_k |b_k|^2}} \tag{6.1.11}$$

In addition one finds with the use of Eq. (6.1.11) that $\langle F_\psi \rangle = \langle \eta_\psi \rangle = 0$. Finally we shall make use of the following correlation functions which are also computed in Appendix F:

$$\langle \eta_\psi(t) \eta_\psi(t') \rangle = \frac{4T}{M_0^2} \sum_k | \int dx f_k(x) \phi_c''(x)|^2 \cos[\omega_k(t-t')] \ , \tag{6.1.12}$$

and

$$\langle F_\psi(t) F_\psi(t') \rangle = \frac{T^2}{4M_0^2} \sum_{k,q} \frac{|A(k,q)|}{\omega_k^2 \omega_q^2} \Big\{ \cos[(\omega_k + \omega_q)(t-t')] + \cos[(\omega_k - \omega_q)(t-t')] \ , \Big\} \tag{6.1.13}$$

where

$$A(k,q) \equiv \int dx \ U'''[\phi_c(x)] \phi_c'(x) f_k(x) f_q(x) \ . \tag{6.1.14}$$

The correlation in Eq. (6.1.13) is different from that of usual random forces since it has a long time tail due to the term when $\omega_k = \omega_q$, whereas the "kink-mass fluctuation" correlation in Eq. (6.1.12) is appreciable only for short times $(t-t')$ since $\omega_k \geq 1$.

To obtain the velocity distribution we solve the "Langevin equation" given in Eq. (6.1.1) with the use of an integrating function which yields

$$\dot{X}(t) = \dot{X}(t_0) e^{-\int_{t_0}^{t} d\tau \ \eta_\psi(\tau)} + \int_{t_0}^{t} d\tau F_\psi(\tau) + O(\psi^3) \ . \tag{6.1.15}$$

Following WS, we turn on the heat bath adiabatically and take $t_0 \to -\infty$ so that $\eta_\psi \to e^{\frac{\delta t}{2}}\eta_\psi$, $F_\psi \to e^{\frac{\delta t}{2}}F_\psi$ with $\delta \to 0$. In squaring Eq. (6.1.15) we encounter the following terms

$$\int_{-\infty}^{t} d\tau \int_{-\infty}^{t} d\tau' \langle \eta_\psi(\tau)\eta_\psi(\tau')\rangle e^{\delta(\tau+\tau')/2} = \frac{4T}{M_0^2}\sum_k \frac{|\int dx f_k(x)\phi_c''(x)|^2}{\omega_k^2} \tag{6.1.16}$$

$$= \frac{T}{M_0} , \tag{6.1.17}$$

where the limit $\delta \to 0$ has been taken without encountering any singularities and Eq. (3.1.15) has been used. Similarly one can show [112]

$$\int_{-\infty}^{t} d\tau \int_{-\infty}^{t} d\tau' \langle F_\psi(\tau)F_\psi(\tau')\rangle e^{\delta(\tau+\tau')} \tag{6.1.18}$$

$$= \frac{T^2}{M_0^2}\sum_{k,q}\frac{|A(k,q)|^2}{\omega_k^2\omega_q^2}\Big[\frac{1}{(\omega_k+\omega_q)^2+\delta^2}+\frac{1}{(\omega_k-\omega_q)^2+\delta^2}\Big] \tag{6.1.19}$$

$$\equiv \alpha T^2 . \tag{6.1.20}$$

In both sine-Gordon and ϕ^4 models [67, 70] $A(k,q) \approx \omega_k^2 - \omega_q^2$; hence, there is no singularity in Eq. (6.1.20) at $\omega_k = \omega_q$ and α is finite. Using these relations we find

$$\langle \dot{X}^2(t)\rangle = \dot{X}^2(0)e^{2T/M_0} + \alpha T^2 + O(T^3) , \tag{6.1.21}$$

which demonstrates the undamped initial velocity. Integrating Eq.(6.1.21) results in [112]

$$\langle X^2(t)\rangle = \dot{X}^2(0)(1+B)(t-t_0)^2 + C\dot{X}^2(0) + (t-t_0)D , \tag{6.1.22}$$

where

$$B = \frac{1}{t-t_0}\int_{t_0}^{t} dt' \int_{-\infty}^{t'} d\tau' \int_{-\infty}^{t'} d\tau \langle \eta_\psi(\tau')\eta_\psi(\tau)\rangle e^{\delta(\tau+\tau')/2} , \tag{6.1.23}$$

$$= \frac{T}{M_0} , \tag{6.1.24}$$

$$C = \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \int_{-\infty}^{t} d\tau' \int_{-\infty}^{\tau'} d\tau \langle \eta_\psi(t'')\eta_\psi(\tau)\rangle e^{\delta(t''+\tau)/2} , \tag{6.1.25}$$

$$= \frac{4T}{M_0^2}\sum_k \frac{|\int dx f_k(x)\phi_c''(x)|^2}{\omega_k^4} , \tag{6.1.26}$$

$$(t-t_0)D = \int\limits_{t_0}^{t} dt' \int\limits_{-\infty}^{t'} dt'' \int\limits_{-\infty}^{t} d\tau' \int\limits_{-\infty}^{\tau'} d\tau \langle F_\psi(t'')F_\psi(\tau)\rangle e^{\delta(t''+\tau)} \ , \tag{6.1.27}$$

and Eqs. (6.1.12-13) have been used. The last term in Eq. (6.1.22) represents the WS result. We evaluate the "diffusion constant" by taking a derivative of Eq. (6.1.22) with respect to time which after some algebra yields

$$D = \frac{T^2}{2M_0^2}\sum_{k,q}\delta\frac{|A(k,q)|^2}{\omega_k^2\omega_q^2}\left\{\frac{1}{[(\omega_k+\omega_q)^2+\delta^2]^2}+\frac{1}{[(\omega_k-\omega_q)^2+\delta^2]^2}\right\} . \tag{6.1.28}$$

To proceed further we make use of the fact [67, 70] that $A(k,q) \approx (\omega_k^2-\omega_q^2)(k-q)$ and that the limit

$$A(k) \equiv \lim_{q\to -k}\frac{A(k,q)}{\omega_k^2-\omega_q^2} \ , \tag{6.1.29}$$

is finite. In the limit as $\delta \to 0$, the pole at $k=-q$ dominates and we have

$$D \approx \frac{2T^2}{M_0^2}\delta\sum_k\frac{|A(k)|^2}{\omega_k^2}\sum_q\frac{1}{(\omega_k-\omega_q)^2+\delta^2} \ , \tag{6.1.30}$$

$$\approx \frac{T^2}{M_0^2}\sum_k\frac{|A(k)|^2}{|k|\omega_k} \ , \tag{6.1.31}$$

which is the result of WS for the diffusion constant. Therefore although we reproduce the result of WS, we obtain the unphysical result alluded to above, namely that the kink's initial velocity is undamped. With a slight modification we include in the next section, the direct thermal coupling to all of the degrees of freedom and obtain the standard Brownian motion result by using a method similar to the Langevin method used above.

6.2 Langevin Approach

Next we study what is the more physically relevant problem in which the system is in contact with a heat bath which we represent by an additive noise term that enters into the full field equation of motion as

$$\Phi_{tt} - \Phi_{xx} + U'(\Phi) = F(x,t) - \epsilon\Phi_t \ , \tag{6.2.1}$$

where a phenomenological damping term has also been added and the Gaussian white noise term has the correlation function [113],

$$\langle F(x,t)\ F(x',t')\rangle = 2\epsilon T\delta(x-x')\ \delta(t-t') \ . \tag{6.2.2}$$

In terms of the perturbation theory presented in section 3.3 we must choose the coupling function $F[\Phi, \Phi_x]$ of that section to be Φ. This in turn leads via Eq. (B.10) of Appendix B to the following second-order equation of motion for $X(t)$

$$(M_0 + \xi)\ddot{X}(t) + (M_0 + \xi)\epsilon\dot{X} + 2\dot{\xi}\dot{X} = F_\psi - G(X,t) \ , \tag{6.2.3}$$

where $G(x,t)$ is the effective thermal noise force for the kink

$$G(X,t) \equiv \int_{-\infty}^{\infty} dx \ \phi_c'(x - X)F(x,t) \ , \tag{6.2.4}$$

has the correlation

$$\langle G(X,t) \ G(X',t')\rangle = 2\epsilon T\delta(t - t') \int_{-\infty}^{\infty} dx \ \phi_c'(x - X)\phi_c'(x' - X) \ . \tag{6.2.5}$$

The fact that this effective noise is not delta-function-correlated in space reflects the extended nature of the kink. In the case in which the nonlinear potential is the sine-Gordon potential we can analytically evaluate this correlation and find it to be

$$\langle G(X,t) \ G(X',t')\rangle = 4\epsilon T \ \delta(t - t')\frac{X - X'}{\sinh(X - X')} \ . \tag{6.2.6}$$

Therefore, although the correlation is not a delta function it is short ranged.

With the aid of an integrating factor $(M_0 + \xi)e^{\epsilon t}$ we obtain for the first integral of Eq. (6.2.3)

$$\dot{X}(t) = \frac{(M_0 + \xi(0))^2}{(M_0 + \xi(t))^2}e^{-\epsilon t}\dot{X}(0) + \frac{1}{(M_0 + \xi(t))^2}e^{-\epsilon t}\int_0^t dt' \ e^{\epsilon t}(M_0 + \xi(t'))\Big[F_\psi - G\Big] \ . \tag{6.2.7}$$

Squaring Eq. (6.2.7) and keeping only lowest order terms we have

$$\langle \dot{X}^2(t)\rangle = e^{-2\epsilon t}\dot{X}^2(0) - e^{-2\epsilon t}\int_0^t dt' \int_0^t dt'' e^{\epsilon(t'+t'')}\langle G(X,t')G(X,t'')\rangle \ . \tag{6.2.8}$$

Since the effective noise terms in Eq. (6.2.8) are evaluated at the same spatial point, we can evaluate the correlation analytically to give us

$$\langle G(X,t')G(X,t'')\rangle = \frac{2\epsilon T}{M_0}\delta(t' - t'') \ . \tag{6.2.9}$$

Making use of the delta function in time we have

$$\langle \dot{X}^2(t)\rangle = e^{-2\epsilon t}\left\{\dot{X}^2(0) - \frac{2T\epsilon}{M_0}\int_0^t dt' e^{2\epsilon t}\right\} , \quad (6.2.10)$$

$$= \frac{T}{M_0} + e^{-2\epsilon t}\left\{\dot{X}^2(0) - \frac{T}{M_0}\right\} . \quad (6.2.11)$$

From Eq. (6.2.11) we see that any kink initial velocity is indeed exponentially damped in time just as a "regular" Brownian particle. Furthermore we see that the kink degree of freedom obeys the equipartition theorem

$$\frac{1}{2}M_0\dot{X}^2 = \frac{1}{2}T , \quad (6.2.12)$$

which agrees with all of our previous results which state that the kink behaves like a Newtonian particle to lowest order.

In order to proceed to higher order, we need to include terms which are of the order ψ^3, that is of order $T^{3/2}$. Referring to Eq. (3.4.7) we see that this means that we must include in Eq. (6.2.3)

$$\frac{\dot{X}^2}{M_0}\int \psi'\phi_c'' , \quad (6.2.13)$$

in addition to ψ^3 terms. The presence of the $\dot{X}^2$ term requires that we find an integrating factor other than that used for the first-order calculation, or deal with this term perturbatively. Both methods are presently under investigation.

6.3 Fokker-Planck Approach

In the preceding section we studied the motion of a kink subject to a fluctuating force by adding phenomenological damping and driving terms to the center of mass equation derived in section 3.4. In this section we first write a Langevin equation for the entire field Φ, derive the corresponding Fokker-Planck equation and then make the transformation to the kink variables. The main benefit of this approach is that we can attempt to answer the question of the approach to equilibrium. Implicit in the work of the previous section is the assumption that the phonons equilibrate more quickly than does the kink degree of freedom. An answer to this question can be found through the Fokker-Planck method.

6.3.1 The Full-Field Fokker-Planck Equation

We begin our derivation of the Fokker-Planck equation by writing the Langevin equation for the entire field $\Phi(x,t)$

$$\Phi_{tt} - \Phi_{xx} + U'[\Phi] + \epsilon\Phi_t = F(x,t) \ , \tag{6.3.1}$$

where x and t are dimensionless space and time variables and the thermal noise term $F(x,t)$ obeys the correlation function

$$\langle F(x,t)\ F(x',t')\rangle = 2\epsilon T\delta(x-x')\delta(t-t') \ . \tag{6.3.2}$$

In order to avoid any assumptions regarding the speed with which the momentum degrees of freedom equilibrate, we write a Fokker-Planck equation for a phase space distribution function $P[\Phi(x,t),\Pi_0(x,t)]$. To this end, we rewrite Eq. (6.3.1) in terms of the field $\Phi(x,t)$ and its conjugate momentum $\Pi_0(x,t)$:

$$\dot{\Phi} = \Pi_0 \tag{6.3.3}$$

$$\dot{\Pi}_0 = \Phi_{xx} - U'[\Phi] - \epsilon\Phi_t + F(x,t) \ , \tag{6.3.4}$$

where as before Φ and Π_0 are canonically conjugate variables. The standard form [108] for the bivariate functional Fokker-Planck equation is

$$\begin{aligned}
&\frac{\partial P(\Phi,\Pi_0;t)}{\partial t} \\
&= \int_{-\infty}^{\infty} dx \Bigg\{ -\frac{\delta}{\delta\Phi}\Big[A_\Phi[\Phi,\Pi_0]P(\Phi,\Pi_0;t)\Big] - \frac{\delta}{\delta\Pi_0}\Big[A_{\Pi_0}[\Phi,\Pi_0]P(\Phi,\Pi_0;t)\Big] \\
&+ \frac{1}{2}\frac{\delta^2}{\delta\Phi^2}\Big[B_{\Phi\Phi}[\Phi,\Pi_0]P(\Phi,\Pi_0;t)\Big] + \frac{1}{2}\frac{\delta^2}{\delta\Pi_0^2}\Big[B_{\Pi_0\Pi_0}[\Phi,\Pi_0]P(\Phi,\Pi_0;t)\Big] \\
&+ \frac{\delta^2}{\delta\Phi\delta\Pi_0}\Big[B_{\Phi\Pi_0}[\Phi,\Pi_0]P(\Phi,\Pi_0;t)\Big]\Bigg\} \ ,
\end{aligned} \tag{6.3.5}$$

where the A and B functions are defined by [108]

$$A_\Phi[\Phi,\Pi_0] = \lim_{\Delta t\to 0}\frac{\langle\Delta\Phi\rangle}{\Delta t} \ , \tag{6.3.6}$$

$$A_{\Pi_0}[\Phi,\Pi_0] = \lim_{\Delta t\to 0}\frac{\langle\Delta\Pi_0\rangle}{\Delta t} \ , \tag{6.3.7}$$

$$B_{\Phi\Phi}[\Phi,\Pi_0] = \lim_{\Delta t\to 0}\frac{\langle(\Delta\Phi)^2\rangle}{\Delta t} \ , \tag{6.3.8}$$

$$B_{\Phi\Pi_0}[\Phi,\Pi_0] = \lim_{\Delta t\to 0}\frac{\langle\Delta\Phi\Delta\Pi_0\rangle}{\Delta t} \ , \tag{6.3.9}$$

$$B_{\Pi_0\Pi_0}[\Phi,\Pi_0] = \lim_{\Delta t\to 0} \frac{\langle(\Delta\Pi_0)^2\rangle}{\Delta t} \ , \tag{6.3.10}$$

and we have omitted the space-time dependence of the fields for notational simplicity. Using Eqs. (6.3.3) and (6.3.4) and the correlation function (6.3.2), it is easy to show that $B_{\Phi\Phi}$ and $B_{\Phi\Pi_0}$ are zero while the others lead to the following equation

$$\begin{aligned}
&\frac{\partial P(\Phi,\Pi_0;t)}{\partial t} \\
&= \int_{-\infty}^{\infty} dx \Bigg\{ -\Pi_0 \frac{\delta}{\delta\Phi} P(\Phi,\Pi_0;t) - \frac{\delta}{\delta\Pi_0}\Big[\Big(\Phi_{xx} - U'[\Phi] - \epsilon\Pi_0\Big) P(\Phi,\Pi_0;t)\Big] \\
&+ \ T\epsilon \frac{\delta^2}{\delta\Pi_0^2} P(\Phi,\Pi_0;t) \Bigg\} \ .
\end{aligned} \tag{6.3.11}$$

As it stands, this equation does not give one much information. However one can easily show that the (time-independent) equilibrium solution may be written as

$$P^{eq}(\Phi,\Pi_0) = e^{-\beta H} \ , \tag{6.3.12}$$

with the Hamiltonian given by

$$H = \frac{1}{2}\Pi_0^2 + \frac{1}{2}\Phi_x^2 + U[\Phi] \ , \tag{6.3.13}$$

which one would expect from equilibrium statistical mechanicals. The most important aspect of this solution is evident when the Hamiltonian is written in terms of the new transformed variables X, p, ψ, π

$$H = \frac{1}{2M_0} \frac{(p + \int \pi\psi')^2}{(1+\xi/M_0)^2} + \int \mathcal{H}_f \ , \tag{6.3.14}$$

where

$$\mathcal{H}_f = \frac{1}{2}\pi^2 + \frac{1}{2}\psi'^2 + V(\psi,\phi_c) \ , \tag{6.3.15}$$

$$V(\psi,\phi_c) = U[\Phi_c + \psi] - \psi U'[\phi_c] - U[\phi_c] \ , \tag{6.3.16}$$

where the background field ψ_0 has been set to zero. As mentioned before we do not have decomposition of the Hamiltonian into terms which are purely kink and purely phonon degrees of freedom. While the absence of such a decomposition complicates the calculations, it leads to some interesting physics. For example, consider the average value which the ψ field attains

$$\langle\psi\rangle \ = \int \mathcal{D}\psi\mathcal{D}\pi\psi e^{-\beta H} \ . \tag{6.3.17}$$

Using the equation which $\dot{X}$ satisifies (Eq. (A.11)),

$$\dot{X} = \frac{p + \int \pi \chi'}{M_0(1 + \xi/M_0)^2} \ , \tag{6.3.18}$$

we can rewrite the Hamiltonian as

$$H = \frac{1}{2} M_0 (1 + \xi/M_0)^2 \dot{X}^2 + \int \mathcal{H}_f \ . \tag{6.3.19}$$

One might object to such a substitution since Eq. (6.3.18) applies only to the stationary path since it is the X equation of motion whereas the functional integrals required in Eq. (6.3.17) involve variations off of this path. The resolution of this apparent problem is that the major contribution to the functional integral occurs along the stationary path, with corrections being of higher order (in temperature). Substitution of Eq. (6.3.19) into Eq. (6.3.17) shows that we have a term which is linear in the ψ field (ξ depends on ψ linearly) with a coefficient proportional to $\dot{X}^2$. This means that in doing the functional integral over ψ one must complete the square in the ψ variable, giving rise to a nonzero equilibrium value for *ψ which depends on $\dot{X}$*, indicating once again the intricate relationship which exists between the kink motion and the "phonons".

6.3.2 Fokker-Planck Equation for the Kink Variables I.

As mentioned above, the Fokker-Planck equation for the full field Φ does not give much information about the kink motion. The obvious thing to do is to make the transformation to the kink and phonon degrees of freedom. One might suspect that since the variable transformation is complex the transformation of the functional derivative operators could be equally complex. This is indeed the case as evidenced by the derivations presented in Appendix G. One of the benefits of using this transformation, however, is that it is a *canonical* transformation and therefore the Jacobian of the transformation is unity. This is an important fact because in the following we shall perform integrals over the phonon degrees of freedom to obtain a Fokker-Planck equation for the reduced distribution function $P(X, p; t)$.

Using these transformation laws we can derive a Fokker-Planck equation for the new phase space distribution function $P[X, p, \psi, \pi; t]$. Since this equation is quite complex and not very illuminating we do not present it. Rather we shall study an equation for a reduced distribution function $P(X, p; t)$. The standard procedure for obtaining a solution for the reduced function [109, 114] is to make a general series expansion for the total distribution function

$$P[X, p, \psi, \pi; t] = \sum_{n=0}^{\infty} P_n(X, p, t) e^{-\beta\pi^2/2} H_n[\pi(x,t)/\sqrt{T}] \alpha_n[\psi(x,t); t] \ , \tag{6.3.20}$$

where the functions H_n are Hermite polynomials and the α_n are functions which need to be determined. However this technique is not a good starting point for our system because we know that our equilibrium solution (6.3.12) has non-separable terms such as

$$p \int \pi\psi' \tag{6.3.21}$$

which cannot be reproduced by the general series representation given in Eq. (6.3.20). Therefore one is forced to make some kind of ansatz for $P[X, p, \psi, \pi; t]$. We base our ansatz on the assumption that the phonon degrees of freedom equilibriate much faster than the kink degrees of freedom, that is we make an adiabatic ansatz. The specific form of the ansatz is

$$P[X, p, \psi, \pi; t] = P(X, p; t) P_{ph}^{eq}[\psi, \pi | X, p] \ , \tag{6.3.22}$$

where the function $P_{ph}^{eq}[\psi, \pi|X, p]$ represents the equilibrium distribution function for the phonons given that the kink degrees of freedom are fixed. One way to obtain this function would be to derive a Fokker-Planck equation for the phonons and solve for the equilibrium distribution function.

6.3.3 Fokker-Planck Equation for the Phonon Variables

The method for deriving the phonon functional Fokker-Planck equation is the same as that used to derive the full field equation. We begin with a Langevin equation for the phonons which is obtained from Eq. (3.4.11)

$$\psi_{tt} - \psi_{xx} + U''[\phi_c]\psi = \mathcal{F}(x, t) - \epsilon \dot{X} \phi_c'(x - X) - \epsilon \psi_t \ , \tag{6.3.23}$$

where

$$\mathcal{F}(x, t) \equiv F(x, t) - \frac{\phi_c'(x)}{M_0} \int \phi_c'(x - X) F(x, t) \ , \tag{6.3.24}$$

with the white noise term $F(x, t)$ having the same correlation as given in section 6.2. The correlation function for the modified noise term $\mathcal{F}(x, t)$ is easily found to be

$$\begin{aligned} \langle \mathcal{F}(x, t)\ \mathcal{F}(x', t') \rangle &= 2T\epsilon \Big[\delta(x - x') - \frac{\phi_c'(x)\phi_c'(x')}{M_0} \Big] \delta(t - t') \ , & (6.3.25) \\ &= 2T\epsilon \delta_\psi(x - x') \delta(t - t') \ , & (6.3.26) \end{aligned}$$

where the δ_ψ term represents a delta function in the subspace perpendicular to the translation mode $\phi_c'(x)$. Using this Langevin equation we can derive the following Fokker-Planck equation for the ψ field

$$\frac{\partial P(\psi, \pi; t)}{\partial t} = \int_{-\infty}^{\infty} dx \left\{ -\pi \frac{\delta}{\delta \psi} P(\psi, \pi; t) - \frac{\delta}{\delta \pi} \Big[\Big(\psi_{xx} - \psi U''[\phi_c] - \epsilon \pi \Big) P(\psi, \pi; t) \Big] \right.$$

$$+T\epsilon\frac{\delta^2}{\delta\pi^2}P(\psi,\pi;t)\Bigg\}\ . \tag{6.3.27}$$

This equation has an equilibrium solution

$$P^{eq} \equiv e^{-\beta H_{ph}}\ , \tag{6.3.28}$$

with H_{ph} given by

$$H_{ph} = \frac{1}{2}\pi^2 + \frac{1}{2}\psi_x^2 + \frac{1}{2}\psi^2 U''[\phi_c]\ . \tag{6.3.29}$$

That this is an equilibrium solution is not too surprising as it is the term from the total Hamiltonian which is clearly due to the phonons. This is in fact the assumption made by WS [67] although to our knowledge they did not give a similar justification.

6.3.4 Fokker-Planck Equation for the Kink Variables II.

With an equilibrium phonon distribution function (6.3.28) in hand we can now proceed to derive the Fokker-Planck equation for $P(X,p;t)$. Following the procedure outlined in section 6.3.2 we substitute the ansatz in Eq. (6.3.22) into the full field Fokker-Planck equation (6.3.11) and carry out the transformation to the kink variables. Since this calculation is a bit tedious we include it in Appendix H from which we obtain

$$\begin{aligned}
&e^{-\beta H_{ph}}\frac{\partial P(X,p;t)}{\partial t} \\
&= e^{-\beta H_{ph}}\Bigg\{\frac{(p+\int\pi\psi')}{M_0(1+\xi/M_0)^2}\frac{\delta P(X,p;t)}{\delta X} \\
&+ \beta\frac{(p+\int\pi\psi')}{M_0(1+\xi/M_0)}P(X,p;t)\int dx\ \phi_c'\Big(\Phi''-U'[\Phi]\Big) \\
&+ \epsilon\frac{\delta}{\delta p}\Big[(p+\int\pi\psi')P(X,p;t)\Big]+\frac{\epsilon}{\beta}\Big(\int\Phi'^2\Big)\frac{\delta^2}{\delta p^2}P(X,p;t)\Bigg\}\ ,
\end{aligned} \tag{6.3.30}$$

with H_{ph} given by Eq. (6.3.29). In writing Eq. (6.3.30) we have omitted all terms which have powers of temperature higher than T, again using the fact that the ψ and π fields, which are assumed to be in equilibrium, are of the order $\sqrt{T}$. Higher order terms are not relevant since the phonon equilibrium distribution derived in the previous section is only approximate.

To obtain a Fokker-Planck equation which does not depend on the phonon variables, we average over the ψ and π fields. Since H_{ph} is quadratic in the both

ψ and π, all odd terms in either of these fields average to zero leaving us with

$$\begin{aligned}\frac{\partial P(X,p;t)}{\partial t} &= -(1+3\frac{\langle\xi^2\rangle}{M_0^2})\frac{p}{M_0}\frac{\delta P(X,p;t)}{\delta X}+\epsilon\frac{\delta}{\delta p}(pP(X,p;t)) \\ &+ M_0\frac{\epsilon}{\beta}(1+\frac{1}{M_0^2}\langle\xi^2\rangle)\frac{\delta^2}{\delta p^2}P(X,p;t)\ . \end{aligned} \tag{6.3.31}$$

where here the angle brackets denote

$$\langle f[\psi,\pi]\rangle = \frac{\int \mathcal{D}\psi\mathcal{D}\pi\ f[\psi,\pi]e^{-\beta H_{ph}}}{\int \mathcal{D}\psi\mathcal{D}\ \pi e^{-\beta H_{ph}}}\ . \tag{6.3.32}$$

Averages similar to those required in Eq. (6.3.31) have been carried out by Miyashita and Maki [115].

In obtaining Eq. (6.3.31) we have made use of the fact that

$$\int \phi_c'\Big[\Phi'' - U'[\Phi]\Big]$$

$$= \int \phi_c'\Big[\phi_c'' + \psi'' - U[\phi_c] - \psi U''[\phi_c] + O[\psi^2]\Big] \tag{6.3.33}$$

$$= \int \phi_c'\Big[\psi'' - \psi U''[\phi_c]\Big] + O[\psi^2]\ , \tag{6.3.34}$$

$$= \int \Big[\phi_c'\psi'' - \psi\frac{d}{dx}U'[\phi_c]\Big] + O[\psi^2]\ , \tag{6.3.35}$$

$$= \int \Big[\phi_c'\psi'' + \psi' U'[\phi_c]\Big] + O[\psi^2]\ , \tag{6.3.36}$$

$$= O[\psi^2]\ , \tag{6.3.37}$$

where we have made repeated use of

$$U'[\phi_c] = \phi_c''\ . \tag{6.3.38}$$

Therefore the second term on the right-hand side of Eq. (6.3.27) is of order

$$T^2 pP(X,p;t)\ . \tag{6.3.39}$$

and has been neglected.

If we further neglect the averaged terms in Eq. (6.3.31), we obtain the bivariate Fokker-Planck equation for a Newtonian particle [108] with momentum p. If p were the momentum of the kink, Eq. (6.3.31) would immediately imply that the kink behaves as a "regular" Brownian particle to lowest order. However, the variable p represents the *total* momentum of the field (see section 3.2) and not the kink momentum, that is

$$\dot{X} = \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)^2}\ . \tag{6.3.40}$$

As before this equation applies only to lowest order since it represents the stationary path, even so it does tell us that the kink momentum $M_0\dot{X}$ and the total momentum p differ by terms of order T, therefore one can interpret Eq. (6.3.31) as stating that the kink behaves as a Brownian particle to lowest order. If we include the averaged terms we see that they have the effect of adding temperature-dependent corrections to the mass and diffusion constant. We have not explicitly performed the functional integrals because it is not yet clear what additional corrections must be included to account for the fact that p is not the kink momentum.

One of the possible approaches to avoid the complications introduced by the fact that p is not the kink momentum is to use a different form of the canonical transformation in which p more closely approximates the kink momentum. This transformation was mentioned in section 3.2 and leads to the following relation between p and $\dot{X}$ [116]

$$p = M_0(1 + \xi/M_0)^2 \dot{X} \; . \tag{6.3.41}$$

Although this form for p still involves the field ψ (through ξ), it does not depend on the momentum π. Compare this with the expression for p obtained from Eq. (3.3.28),

$$p = M_0(1 + \xi/M_0)^2 \dot{X} - \int \pi\psi' \; . \tag{6.3.42}$$

Clearly the difference is the addition of the momentum carried by the phonon field. The factors of $1 + \xi/M_0$ which appear in both expressions represent a renormalization of the kink mass due to the phonon field ψ. Since the transformation which leads to Eq. (6.3.42) is also canonical, it can serve as a basis for our Fokker-Planck equation. Efforts which utilize this transformation are currently underway.

6.3.5 Higher Order Terms

Now that we have a lowest order result for the kink distribution function, we can continue to higher order. This involves writing a Fokker-Planck equation for the phonons using the lowest-order kink distribution function in the ansatz. When this equation is obtained we plan to calculate the time required to achieve equilibrium and confirm our ansatz that the phonons equilibrate more quickly than the kink. These calculations are currently in progress.

Another route to higher order terms would be to start with a phonon equilibrium distribution function which is valid to higher order in temperature. The rather obvious choice is the *exact* equilibrium distribution function itself

$$P_{ph}^{eq}[\psi, \pi | X, p] = e^{-\beta H} \; . \tag{6.3.43}$$

Again making the ansatz

$$P[X, p, \psi, \pi] = P(X, p; t) P_{ph}^{eq}[\psi, \pi | X, p] \; , \tag{6.3.44}$$

we easily derive the following equation for P(X,p;t):

$$
\begin{aligned}
& e^{-\beta H}\frac{\partial P(X,p;t)}{\partial t} \\
= \;& e^{-\beta H}\Big\{ - \frac{(p+\int \pi\psi')}{M_0(1+\xi/M_0)^2}\frac{\delta P(X,p;t)}{\delta X} \\
+ \;& \epsilon\frac{\delta}{\delta p}\Big[pP(X,p;t)\Big] + \frac{\epsilon}{\beta}\Big(\int \Phi'^2\Big)\frac{\delta^2}{\delta p^2}P(X,p;t)\Big\} \;, \qquad (6.3.45)
\end{aligned}
$$

where we have made use of the fact that

$$
\int dx \; \Pi_0 \Phi' = p \; . \qquad (6.3.46)
$$

Notice that this equation does not contain a term similar to the second term on the right-hand side of Eq. (6.3.30), which we eventually showed was of order T^2. This term does not occur because in using the exact equilibrium solution, much cancellation occurs. Doing the functional averages over the phonon fields we obtain

$$
\begin{aligned}
\frac{\partial P(X,p;t)}{\partial t} = \;& -(1+3\frac{\langle\xi^2\rangle}{M_0^2})\frac{p}{M_0}\frac{\delta P(X,p;t)}{\delta X} + \epsilon p\frac{\delta}{\delta p}P(X,p;t) \\
+ \;& M_0\frac{\epsilon}{\beta}(1+\frac{1}{M_0^2}\langle\xi^2\rangle)\frac{\delta^2}{\delta p^2}P(X,p;t) \; . \qquad (6.3.47)
\end{aligned}
$$

This is nearly identical with the result obtained in the previous section, the difference occuring in the second term in which the momentum derivative operates only on the distribution function $P(X,p;t)$ instead of on the product $pP(X,p;t)$. This results in an equation which is *not* a Fokker-Planck equation. Indeed the function $P(X,p;t)$ is no longer a probability distribution function since it is not normalizable. To see this explicitly, note that since we used the exact equilibrium solution in our ansatz, the "equilibrium" solution $P(X,p;\infty)$ must be unity, a fact which is easily checked. Of course the entire distribution function $P[X,p,\psi,\pi]$ is normalizable and the integral of $P[X,p,\psi,\pi]$ over X,p,ψ,π is conserved for all time because it satisifies a Fokker-Planck equation, which is in divergence form. Once again it would be useful to have a momentum variable p which represents the kink momentum, so to that end the alternate form of the canonical transformation should be implemented. Then one can derive an equation similar to Eq. (6.3.47) and attempt to solve it via standard separation-of-variables techniques.

6.3.6 Constant Driving Force

So far we have considered only the undriven system in which we have found that the kink will execute Brownian motion to lowest order. A physically more relevant situation involves the inclusion of a constant driving force which will cause the kink to move at some finite velocity, contributing to various transport quantities such as mobility.

Denoting the strength of the constant driver by E_0, the full field equation becomes

$$\Phi_{tt} - \Phi_{xx} + U'[\Phi] = E_0 - \epsilon\Phi_t + F(x,t) \ , \qquad (6.3.48)$$

where as before the fluctuating force $F(x,t)$ represents delta-function- correlated white noise. The Fokker-Planck equation associated with this Langevin equation is

$$\begin{aligned} &\frac{\partial P(\Phi,\Pi_0;t)}{\partial t} \\ &= \int\limits_{-\infty}^{\infty} dx \Bigg\{ -\Pi_0 \frac{\delta}{\delta\Phi} P(\Phi,\Pi_0;t) - \frac{\delta}{\delta\Pi_0}\Big[\Big(\Phi_{xx} - U'[\Phi] + E_0 - \epsilon\Pi_0\Big)P(\Phi,\Pi_0;t)\Big] \\ &+ \ T\epsilon\frac{\delta^2}{\delta\Pi_0^2}P(\Phi,\Pi_0;t)\Bigg\} \ . \qquad (6.3.49) \end{aligned}$$

We would like to proceed as in the undriven case and derive a Fokker-Planck equation for a reduced distribution function $P(X,p;t)$ for the kink variables. The first step is to find a steady-state (cf. equilibrium solution for the undriven case) solution for Eq. (6.3.48). Formally $e^{-\beta H}$ with H given by

$$H = \frac{1}{2}\Pi_0^2 + \frac{1}{2}\Phi_x^2 + U[\Phi] - E_0\Phi \ , \qquad (6.3.50)$$

is a solution to Eq. (6.3.48). However, this Hamiltonian is unbounded from below due to the term linear in Φ and is therefore physically unacceptable. At this point we realize that the addition of a constant force greatly modifies the problem and that before we proceed, we should understand these modifications and their implications.

To understand these some of these modifications, it is useful to refer once again to the pendulum chain. For example, a constant torque E_0 on the pendulum chain will cause all of the pendula to attain a new equilibrium position Φ_0 given by

$$U'[\Phi_0] = E_0 \ . \qquad (6.3.51)$$

One of the obvious ways to account for this deviation is to use a nonzero ψ_0 field. A more subtle method would be to change the definition of what is meant by a kink, a possibility which has already been examined in section 5.4. In either case, one must also deal with infinite energy terms or for the finite system considered below, terms which diverge with the length of the system. This divergence can be removed by a suitable subtraction from the Hamiltonian.

In addition to a constant deformation of the field, we can expect to see a nonsymmetrical change in the kink waveform [102], that is the kink will achieve a nonzero “polarization” [37]. This change in the kink profile will be well-localized about the kink center and move with the velocity of the kink. Again this deformation could be included in the definition of the kink, or we could account for it through the ψ_0 field, however since the kink will be moving (either at or approaching a terminal velocity), ψ_0 would have to depend on time which complicates matters more.

It might seem that the matters discussed in the previous two paragraphs are more relevant to the dynamics of a kink without the thermal force present. However in writing a Fokker-Planck equation for the kink variables we will again need to make an adiabatic ansatz in which we freeze the kink degrees of freedom and postulate the equilibrium distribution function of the phonons. Since this distribution function depends on the configuration of the field, we need some detailed knowledge of the (deformed) kink profile.

Another feature which requires closer attention in the driven case is the question of boundary conditions. In the undriven case we glossed over this point because the system is translationally invariant. In anticipation of dealing with the added complication of the motion of a kink in a position-dependent potential under the influence of thermal forces [117, 118, 119, 120, 121], we consider some of the consequences of applying the proper boundary conditions. Before a specific boundary condition is chosen, we must first realize that in order to properly account for the correct number of degrees of freedom [75, 48], we must deal with a system of finite length and take the thermodynamic limit at the end of the calculation. The boundary condition which is most easily dealt with is the periodic one (mod (2π)). Having a system of finite length subject to periodic boundary conditions requires us to use the kink solutions [122, 123] and linearized phonons appropriate to this system. The analytic solutions for the kink solutions on the finite line are expressable in terms of Jacobi ellpitic functions [122] whereas the phonons can be written in terms of theta functions [33].

One can obtain a physical picture of the periodic boundary conditions by imagining the pendulum chain “bent” into a circle, connecting the first and last pendula together. In traversing this circle the angular deviation of the pendula changes smoothly from zero to 2π (=0) representing the kink. An alternate method of viewing the periodic system is to consider a “kink lattice”. In this case we imagine a long pendulum chain divided into cells of length l. Each cell contains a kink, however this time the total angular deviation experienced in going from the beiginning to the end of the kink can be less than 2π [124]. An additional feature of this kink lattice approach is the presence of two phonon bands separated by a gap [124]. The first of these bands represents vibrations of the kink lattice itself, the zero frequency mode again representing a rigid translation of the entire lattice. The second band is similar to the phonons described in section 4.1. In the thermodynamic limit this first band becomes negligible and we approach the dispersion relation which applies to the infinite system.

The stage is now set for carrying out the calculations begun in this chapter to higher order. Not only can the temperature dependent mass and diffusion coefficients be calculated, but the question of the approach to equilibrium can now be attacked. In addition, many of the added difficulties which enter the problem when a constant driver is added have been examined and possible solutions have been considered. As a final step, one might try to use the variable transformation to study the more general problem of a Boltzmann equation.

Chapter 7

Kink-Antikink Collisions in ϕ^4

So far we have dealt with the use of a single collective coordinate which represents the center of mass of a Klein-Gordon kink. Because we have a canonical transformation from the original field variables to the "kink" variables, this method is on very firm ground and therefore is expected to yield reasonable results. However, the rigor lent by this transformation is also a weakness since one cannot expect to find the appropriate canonical transformation for an arbitrary system (assuming one even exists). Since this canonical transformation is based on the physically reasonable decomposition

$$\Phi(x,t) = \phi_c(x - X(t)) + \chi(x - X(t), t) \ ,$$

one would hope that similar physically reasonable ansätze which do not necessarily represent canonical transformations would also prove useful. In order to explore this possibility, we consider in this chapter the use of two collective coordinates to model the kink-antikink collisions in ϕ^4 field theory. We begin by reviewing the behavior observed in the numerical simulation of the PDE. In section 7.2 we outline collective coordinate approaches which have been used and introduce an ansatz based on two collective coordinates. Section 7.3 contains plots and limiting analytic forms for the coordinate-dependent masses and potential which one obtains from the averaged Lagrangian. The equations of motion are presented and their numerical solution discussed in section 7.4. These solutions of the equations indicate that the ansatz breaks down when the two kinks collide. The limiting case in which the kinks are very close is examined in section 7.5 in which we find that one of the coordinates undergoes very rapid changes as the separation between the kinks goes to zero. A new ansatz based on the original one but which includes "relativistic" terms is proposed in section 7.6. Simulations of the equations of motion which result from this ansatz are currently being carried out.

7.1 Observed Phenomena in Numerical Simulations

As mentioned in the introduction, the ϕ^4 system is not integrable but it does possess exact kink(+) and antikink(-) solutions

$$\phi_K(x) = \pm \tanh \frac{(x - x_0)}{m\sqrt{2}} \ . \tag{7.1.1}$$

Since the ϕ^4 system is not integrable but possesses solitary wave solutions (not solitons), it of interest to study the interaction between two such solitary waves. Several investigators [125, 126, 127, 128, 129, 130, 131, 132] have studied the collision of a kink and antikink by the direct numerical integration of the PDE. Initial studies showed that when the kink velocities were above some critical value v_c, the kinks scattered off of one another inelastically transferring energy to other modes of the system such as radiation ("phonons"). For velocities less than v_c the kinks were found to form a bound state, again transferring some energy into the radiation degrees of freedom. Further investigation showed that for certain velocity intervals $v_i < v < v_j < v_c$ (see Figure 7.1) the kinks did not form a bound state but scattered off to $\pm\infty$. Similar phenomena have been observed in other nonintegrable systems such as the parametrically modified sine-Gordon [50] and double sine-Gordon [133] systems. These "resonance windows" have been quantitatively explained by Campbell et al. [15] in terms of an exchange of energy between the kink translational energy and a localized mode known as the "shape mode", which can be thought of as representing a modification of the kink solution. The basic idea is that when the kinks first collide, there is an energy transfer into the shape mode. The kinks then move apart, but not having enough energy to overcome the attractive potential which exists between them (i.e. some energy was given to the shape mode), they fall back toward one another. When they collide again, the energy in the shape mode can be transferred back to the translational motion if the time between the collisions obeys the following resonance condition:

$$\omega_2 T = \delta + 2n\pi \ ,$$

where $\omega_2 = \sqrt{3}/2$ is the frequency of the shape mode. Such a transfer of energy allows the kink and antikink to overcome the attractive potential and escape to infinity. Using these ideas Campbell et al. have been able to predict the bounds v_i of the resonance windows which are in good agreement with the results obtained from the numerical simulations. The analysis, however treats the collision as a "black box" and does not provide any details of the collision as do the PDE simulations.

Figure 7.1: Results of a numerical simulation showing the final kink velocity after a ϕ^4 $K\bar{K}$ collision as a function of the initial kink velocity. A final velocity of zero indicates the formation of a bound state. Taken from Ref. 15 with the permission of the authors.

7.2 Collective Coordinate Approaches

To gain an understanding of the collision process without solving the PDE, several collective coordinate methods have been put forth to study the $K\bar{K}$ collisions. Although Aubry [130] was the first to observe the resonance structure, Kudryavtsev [125] was the first to implement coordinates which showed that the effective potential between the kink and antikink was attractive. In another early study, Sugiyama [131] introduced collective coordinates which represent the center of mass of the kinks and the amplitudes of the shape mode and radiation degrees of freedom. His analysis was purely analytic, producing an attractive potential in which the kinks moved and a solution for the shape mode coordinate which exhibited harmonic oscillations.

A collective coordinate ansatz very similar to that used by Sugiyama was introduced by Jeyadev and Schrieffer [134]. In the notation established in section 3.1 the ansatz has the form

$$\begin{aligned}\Phi_A(x,t) &= 1+\tanh y_- - \tanh y_+ \\ &+ A(t)\left[f_{b,2}(y_-)\cos\frac{\omega_{b,2}(t-\beta x)}{\sqrt{1-\beta^2}} - f_{b,2}(y_+)\cos\frac{\omega_{b,2}(t+\beta x)}{\sqrt{1-\beta^2}}\right] \\ &+ \sum_k B_k(t)\left[f_k(y_-)\cos\frac{\omega_k(t-\beta x)}{\sqrt{1-\beta^2}} - f_k(y_+)\cos\frac{\omega_k(t+\beta x)}{\sqrt{1-\beta^2}}\right] \quad (7.2.1)\end{aligned}$$

with the definitions

$$y_\pm = \frac{x\pm\alpha(t)}{\sqrt{2}\sqrt{1-\beta^2}} \quad , \quad \beta=\dot{\alpha} \; . \qquad (7.2.2)$$

Substitution of this ansatz into the Lagrangian density and integration over space yields a Lagrangian which depends on the collective coordinates $\alpha(t), A(t), B_k(t)$ and their time derivatives. The resulting equations of motion are quite complex when all of the relativistic and phonon terms are included and therefore only the lowest order terms in the velocity were included in the simulations, the phonon terms being dropped entirely. The numerical results based on this model showed that the kinks attained relativistic velocities (in fact β became > 1). When this occurred the amplitude of the shape mode also became large, which in turn caused the velocity to diverge.

A slightly different ansatz

$$\Phi_A(x,t) = \frac{m}{\sqrt{\lambda}}\left\{1-\tanh\Big[\frac{my_0(x-x_0)}{\sqrt{2}}\Big] + \tanh\Big[\frac{my_0(x+x_0)}{\sqrt{2}}\Big]\right\} \; . \qquad (7.2.3)$$

was put forth by Campbell et al. [15]in their original work describing the PDE simulations . This ansatz represents a kink-antikink pair moving in opposite directions according to the center of mass variable $x_0(t)$ (see Figure 7.2). Like the

Figure 7.2: Schematic representation of the ansatz in Eq. (7.2.3)

previous ansätze, there is a collective coordinate x_0 which describes the center of mass motion of the kinks. The y_0 coordinate takes the place of the shape mode contribution by allowing the width of the kinks $(1/y_0)$ to vary as a function of time. The x_0 collective coordinate is much like the X coordinate used in the previous chapter in that it is a result of the translational invariance of the original equations. The y_0 coordinate, however appears merely as a parameter in the ansatz. Equation (7.1.1) is a solution of the field equations only for $y_0 = 1$, x_0 being able to take on any value. Therefore the y_0 coordinate has been termed a "parametric collective coordinate" [42, 15] while the x_0 coordinate is a "linear collective coordinate". No matter what the values of x_0 and y_0, the ansatz given in Eq. (7.2.3) is not an exact solution of the original field equations and it does not represent a canonical transformation to a new set of variables; however in view of the explanation of the resonance windows given by Campbell et al., it is certainly a reasonable choice.

Proceeding along the same lines as Jeyadev and Schrieffer [134] , we substitute this ansatz into the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\Big(\frac{\partial_t \Phi_A}{\partial t}\Big)^2 - \frac{1}{2}\Big(\frac{\partial_x \Phi_A}{\partial t}\Big)^2 + \frac{\lambda}{4}(\Phi_A^2 - \frac{m^2}{\lambda})^2 \ , \tag{7.2.4}$$

and integrate over x, yielding a Lagrangian

$$\begin{aligned} L(x_0, \dot{x}_0, y_0, \dot{y}_0) &= \frac{1}{2} m_1(x_0, y_0)\dot{x}_0^2 + m_2(x_0, y_0)\dot{x}_0\dot{y}_0 + \frac{1}{2} m_3(x_0, y_0)\dot{y}_0^2 \\ &- V(x_0, y_0) \ , \end{aligned} \tag{7.2.5}$$

where the expressions for the masses and potentials along with some useful limits are given in Appendix I. One of the interesting features of this Lagrangian and the associated Hamiltonian is the appearance of coordinate dependent masses. Since the masses depend on the coordinates, we cannot use the usual potential energy arguments to give us an idea of what the solution is. One might ask whether one can somehow make a transformation to a new set of variables x_0', y_0' in terms of which the masses are coordinate independent. Such a procedure is available for systems with only one coordinate [135] and merely requires finding the transformation to a new variable $q(q')$ such that

$$m(q)\dot{q}^2 = \tilde{m}\dot{\tilde{q}}^2 \ . \tag{7.2.6}$$

This equation is easily integrated to yield

$$\tilde{q}(q) - \tilde{q}(q_0) = \int_{q_0}^{q} dq' \sqrt{\frac{m(q')}{\tilde{m}}} \ . \tag{7.2.7}$$

The analogous procedure for our system involves first diagonalizing the kinetic energy terms in Eq. (7.2.5), followed by the integration of a coupled set of ODEs.

Since we are not assured of finding a solution of these equations (even numerically), this method shows little promise. Since we have to deal with the coordinate dependent masses and potentials, it is helpful to become acquainted with this dependence.

7.3 The Potential $V(x_0, y_0)$ and Masses $m_i(x_0, y_0)$

As mentioned above, the effective mutual potential experienced by the kink and antikink is attractive as is shown in Figure 7.3. One might argue that since the masses depend on the coordinates, interpreting the effective potential as attractive is not valid; however one can always restrict the coordinates to a small enough range so that the masses are essentially constant. The linear behavior in the potential for values of $x_0 < 0$ represent the fact that the kinks cannot pass through one another to infinity. One can understand this by considering the field amplitude for a configuration in which the kinks have passed through one another (see Figure 7.2). In the segment of length L, the field amplitude is a constant ϕ_0. The energy content of this segment is $(\phi_0^2 - 1)^2 L$ which diverges linearly with L as shown in Figure 7.3.

The masses $m_1(x_0, y_0), m_2(x_0, y_0)$ and $m_3(x_0, y_0)$ are plotted in Figures 7.4-7.6. (It should be noted that in all of the plots, the minimum value of y_0 plotted is not 0. The scale begins at $y_0 = 0$ because the graphics package used automatically scales the plots so that the numbers on the scale are "round" numbers.) For large x_0, m_1 approaches a constant value which is easily shown to be (see Appendix I)

$$m_1(x_0, y_0) \longrightarrow \frac{8}{3}\sqrt{2}m^3 y_0/\lambda \ , \tag{7.3.1}$$

which is twice the mass of a single kink. Figure 7.5 shows that for small x_0, m_2 vanishes linearly while m_3 vanishes quadratically. One of the consequences of these vanishing masses is that for $x_0 = 0$ the kinetic energy is entirely carried by the translation of the kinks. More importantly, we see from the Lagrangian that for m_2 and m_3 equal zero, the value of $\dot{y}_0$ is arbitrary, a fact that will give rise to numerical trouble when the equations of motion are integrated. Finally we note that the mass m_3 shows a divergence as the y_0 coordinate approaches zero. All of the limiting properties of the potential and masses are summarized in Table 7.1.

From the analytic expressions for the masses and potentials given in Appendix I one might expect that as either the x_0 or y_0 coordinates tends to zero, these quantities might not be computed accurately since both the numerator and denominator tend to zero. To avoid such problems the limits of the potentials and masses were taken analytically. With the aide of the symbolic manipulation program MACSYMA [136] the Taylor series were taken up to and including terms

Figure 7.3: The effective potential $V(x_0, y_0)$.

Figure 7.4: The mass $m_1(x_0, y_0)$.

Figure 7.5: The mass $m_2(x_0, y_0)$.

Figure 7.6: The mass $m_3(x_0, y_0)$.

	$z_0 \to 0$	$z_0 \to \infty$
$V_1(x_0, y_0)$	$\frac{8\sqrt{2}m^5x_0^2y_0^3}{15\lambda}$	$\frac{2\sqrt{2}m^3y_0}{3\lambda}$
$V_2(x_0, y_0)$	$\frac{8\sqrt{2}m^5x_0^2y_0}{3\lambda}$	$\frac{2\sqrt{2}m^3}{3\lambda y_0}$
$m_1(x_0, y_0)$	$\frac{8\sqrt{2}m^3y_0}{3\lambda}\left[1 - \frac{2m^2x_0^2y_0^2}{5}\right]$	$\frac{8\sqrt{2}m^3y_0}{3\lambda}$
$m_2(x_0, y_0)$	$\frac{8\sqrt{2}m^3x_0}{3\lambda}\left[\frac{1}{2} - \frac{2m^2x_0^2y_0^2}{5}\right]$	0
$m_3(x_0, y_0)$	$\frac{8\pi^2\sqrt{2}m^3x_0^2}{45\lambda y_0}$	$\frac{8m}{\sqrt{2}\lambda y_0^3}\frac{1}{3}\left(\frac{\pi^2}{3} - 1\right)$

Table 7.1: Limiting values for the potentials and masses for z_0 approaching 0 and ∞. The total potential V is the sum of V_1 and V_2. Analytic expressions for V_1 and V_2 are given in Appendix I.

on the order of z_0^{10} with $z_0 = mx_0y_0/\sqrt{2}$. To assure a smooth transition from the analytic to Taylor series expressions both quantities were computed for a variety of small values of z_0. For z_0 of the order of 0.01, the expressions gave the same values to *at least* 9 significant digits. As a further check on the analytic forms given in Appendix I, the integral expressions were numerically evaluated. Again we found the analytic and numerically integrated values of the masses and potential agree to *at least* 9 significant digits.

7.4 Equations of Motion

Application of the Euler-Lagrange method yields the following equations of motion for x_0 and y_0:

$$\begin{aligned} m_1\ddot{x}_0 + m_2\ddot{y}_0 &+ \frac{1}{2}\frac{\partial m_1}{\partial x_0}\dot{x}_0^2 \\ &+ \frac{\partial m_1}{\partial y_0}\dot{x}_0\dot{y}_0 + \frac{\partial m_2}{\partial y_0}\dot{y}_0^2 - \frac{1}{2}\frac{\partial m_3}{\partial x_0}\dot{y}_0^2 + \frac{\partial V}{\partial x_0} = 0 \ , \qquad (7.4.1) \end{aligned}$$

$$m_3\ddot{y}_0 + m_2\ddot{x}_0 + \frac{1}{2}\frac{\partial m_3}{\partial y_0}\dot{y}_0^2$$

Figure 7.7: Position (solid) and velocity (dashed) for a "wobbling kink" solution.

$$+ \quad \frac{\partial m_3}{\partial x_0}\dot{x}_0\dot{y}_0 + \frac{\partial m_2}{\partial x_0}\dot{x}_0^2 - \frac{1}{2}\frac{\partial m_1}{\partial x_0}\dot{x}_0^2 + \frac{\partial V}{\partial y_0} = 0 \ . \qquad (7.4.2)$$

In general this set of coupled equations must be solved numerically; however, an analytic solution can be found in the limiting case in which x_0 approaches ∞. Guided by the numerical integration of the PDE, one is led to search for a solution in which the velocity of the kinks oscillates about a constant value. Such a solution has been obtained by Campbell [137], with the period of oscillation given by

$$T = 2\pi\sqrt{\left(\frac{\pi^2}{6} - 1\right)\left(1 - v_f^2\right)} \approx 5.04\sqrt{1 - v_f^2} \ , \qquad (7.4.3)$$

where v_f is the mean of the final velocity. This analytic result proves to be a good check of the numerical integrator. In Figure 7.7 we present results of the numerical integration of Eqs. (7.4.1-2) for initial conditions

$$x_0 = 20 \quad , \quad \dot{x}_0 = 0.2 \quad , \quad y_0 = 1 \quad , \quad \dot{y}_0 = 0 \ . \qquad (7.4.4)$$

Making a rough measurement from this graph we find that the oscillation period is 4.94 compared with 4.94 as computed from Eq. (7.4.3) with v_f approximated by 0.196.

In the above example we started the kink and antikink moving away from each other so that a comparison could be made with analytic results (initial conditions in which the kink and antikink collided yield simliar results). Figure 7.8 shows the integrated values of the variables and their time derivatives for initial conditions for which the kink and antikink collide. Initially the kink and antikink travel toward each other with initial velocities of -0.2 and +0.2 respectively. When the kink and antikink are approximately 3 units apart they begin to accelerate towards one another under the influence of their mutually attractive potential. At x_0 the the kinks very abruptly bounce off of one another after which they move apart, their velocities experiencing small oscillations which represent a transfer of energy into the oscillating width (shape mode) of the kinks (see Figure 7.8). From Figure 7.1 we see that for the initial velocity of -0.2, the kinks should indeed eventually scatter to $\pm\infty$; however the numerical simulations of the PDE indicate that the kink and antikink actually pass through one another ($x_0 < 0$) before they turn around and move off to $\pm\infty$. Furthermore, before they separate to $\pm\infty$, they should experience a second collision in which the energy given to the shape mode oscillation is returned to the translational motion allowing them to escape. This asumes that the ansatz will capture all of the details of the collision which one cannot expect since we allow for no radiation degrees of freedom. However, one would hope to be able to capture the resonance windows. Additional simulations with initial velocities which are not in the windows, that is, initial velocities for which we should see a bound state formed, also show this type of hard bounce. Finally in Figure 7.8 we see the y_0 coordinate is well behaved until it increases rapidly when x_0 approaches 0. The oscillations which occur after this sharp spike again reflect the sharing of energy between the translational kinetic energy and the energy associated with the changing kink width.

In Figure 7.9 we examine more closely the region for which the “hard bounce” seen in Figure 7.8 occurs. The initial conditions used for this run correspond to the values of the variables and their derivatives at $t = 42$ in Figure 7.8. Here we see that the hard bounce at $x_0 = 0$ in fact occurs smoothly on a smaller time scale. Examination of the plots of the y_0 coordinate and its derivative on this finer time scale are further causes of concern since a y_0 value of 40 represents extremely sharp kinks, another feature which is not observed in the PDE simulations. Another interesting feature of these plots is that the kink velocities approach -1 and then turn around, echoing the results of Jeyadev and Schrieffer [134]. The fact that the velocity gets so close to its relativistic limit of -1 seems to indicate that a “relativistic” treatment of the problem is in order. This possibility is outlined in section 7.6.

Given these rather unexpected and somewhat unphysical results, one immediately questions the accuracy of the codes used to integrate the equations. We have already mentioned in section 7.3 that extreme care has been taken in the eval-

Figure 7.8: The kink position x_0 (solid) and inverse width y_0 (solid) along with their time derivatives (dashed) as a function of time.

Figure 7.9: Blow up of the "hard bounce" region of Figure 7.8

Figure 7.10: Hamiltonian vs. time during the bounce.

uation of the potential, masses, and their derivatives, and therefore they can be ruled out as a possible problem. Next one questions the accuracy of the numerical integrator used. Since a Hamiltonian exists for this problem, namely

$$\begin{aligned} H(x_0, \dot{x}_0, y_0, \dot{y}_0) &= \frac{1}{2} m_1(x_0, y_0)\dot{x}_0^2 + m_2(x_0, y_0)\dot{x}_0\dot{y}_0 + \frac{1}{2} m_3(x_0, y_0)\dot{y}_0^2 \\ &+ V(x_0, y_0) \ , \end{aligned} \tag{7.4.5}$$

we can monitor it as a function of time as a check on the numerical integrator. In Figure 7.10 we plot the Hamiltonian as a function of time corresponding to the variables plotted in Figure 7.9. From this plot we see that the Hamiltonian is indeed quite well conserved, although there is obviously something drastic happening when $x_0 = 0$. An even greater accuracy, up to about 1 part in 10^{-9} can be achieved by decreasing the error tolerances of the numerical integrator. The fact that the Hamiltonian is conserved so well, coupled with the fact that the code accurately reproduces the oscillation period, indicates that the equations have been coded properly and that the integrator is working. This leads us to consider what features of the ODEs could cause such behavior, or more importantly, to find the root of the problem in the original ansatz.

7.5 Limiting Analysis: $x_0 \to 0$

Since the problem occurs for small values of the x_0 coordinate, it is useful to examine the equations of motion in this limiting case. Using the results from Table 7.1, one arrives at the following equations after a bit of algebra:

$$\ddot{x}_0 \approx x_0\left[Dm^2y_0^2(\dot{x}_0^2-1)+\frac{C}{y_0^2}-2m^2\right]+O(x_0^2)\ , \tag{7.5.1}$$

$$x_0\ddot{y}_0 \approx -2\dot{x}_0\dot{y}_0+Ey_0^3x_0(\dot{x}_0^2-1)+O(x_0^2)\ , \tag{7.5.2}$$

with the constants C, D and E given by

$$C = \frac{\pi^2}{15}\approx 0.65 \tag{7.5.3}$$

$$D = \frac{2}{5}\left(\frac{4C-3}{4C-1}\right)\approx -0.09 \tag{7.5.4}$$

$$E = \frac{2}{5}(C-.25)^{-1}\approx 0.98\ . \tag{7.5.5}$$

Since these equations are valid only for small x_0, one cannot divide the equation for y_0 by x_0. The numerical integrator used to solve the equations of motion is an algebraic-differential equation solver, which means that the form for the y_0 equation given in Eq. (7.5.2) is what is used in the code. Even though the integrator can handle such a potential singularity, it is clear from Eq. (7.5.2) that we can expect some very rapid changes in the y_0 coordinate as $x_0 \to 0$.

Another interesting feature of the limiting equations is the appearance of the factors $\dot{x}_0^2 - 1$. Recall that the velocity in Figure 7.9 reached a minimum value of -1 before turning around. Since this behavior has been observed for initial velocities other than that shown in Figure 7.9, one is led to look for zeroes of the right-hand side of Eq. (7.5.1) (zeroes in $\ddot{x}_0$ correspond to "turning points" in $\dot{x}_0$). Such a turning point would occur for $\dot{x}_0^2 = 1$ if

$$\frac{C}{y_0^2} = 2m^2\ . \tag{7.5.6}$$

In the simulations we have taken $m = \lambda = 1$ (these choices were made so that direct comparisons could be made with the PDE simulations [15]), so Eq. (7.5.6) requires that $y_0 \approx 0.57$, a condition which does not hold in Figure 7.9 and in other simulations. Presently an effort is being made to search for zeroes of the right-hand side of the exact x_0 equation to see if a turning point for $\dot{x}_0^2 = 1$ is a generic feature.

From the limiting forms of the equations of motion, we see that there must be some very rapid behavior near $x_0 = 0$. This fact is further supported by an examination of the Hamiltonian surface on which the motion must occur. The Hamiltonian surface is a three dimensional surface embedded in the four dimensional state space $(x_0, \dot{x}_0, y_0, \dot{y}_0)$. The most convenient method of examining such a surface is to fix one of the coordinates and examine a two dimensional section of the three dimensional surface. To compute values on this surface, it is easiest to solve for either $\dot{x}_0$ or $\dot{y}_0$ using the quadratic formula which yields

$$\dot{x}_0(x_0, y_0, \dot{y}_0; H_0) = -m_2\dot{y}_0 \pm \frac{1}{m_2}\sqrt{m_2^2\dot{y}_0^2 - 2m_1\left(\frac{1}{2}m_3\dot{y}_0^2 + V - H_0\right)} , \quad (7.5.7)$$

$$\dot{y}_0(x_0, y_0, \dot{x}_0; H_0) = \frac{-m_2}{m_3}\dot{x}_0 \pm \frac{1}{m_3}\sqrt{m_2^2\dot{x}_0^2 - 2m_3\left(\frac{1}{2}m_1\dot{x}_0^2 + V - H_0\right)} . \quad (7.5.8)$$

Using the limiting forms given in Table 7.1 we can compute the values that $\dot{y}_0$ must take as $x_0 \to 0$:

$$\dot{y}_0(x_0, y_0, \dot{x}_0; H_0) \to \frac{\alpha y_0}{x_0}\left[-\dot{x}_0 \pm \sqrt{\dot{x}_0^2 - \beta\left(\frac{m_1\dot{x}_0^2}{2} + V - H_0\right)}\right] , \quad (7.5.9)$$

with α and β given by

$$\alpha = \frac{15}{2\pi^2} , \quad (7.5.10)$$

$$\beta = \frac{\pi^2}{5\sqrt{2}m^3 y_0} . \quad (7.5.11)$$

This limiting form for $\dot{y}_0$ tells us that for finite $\dot{x}_0$, unless

$$\frac{1}{2}m_1\dot{x}_0^2 + V - H_0 = 0 , \quad (7.5.12)$$

$\dot{y}_0$ will diverge as x_0 approaches 0. If Eq. (7.5.12) is satisfied, we find that $\dot{y}_0$ is zero. This type of behavior in $\dot{y}_0$ is confirmed in Figure 7.9. If we plot the values of $\dot{y}_0$ as computed from the exact quadratic formula given in Eq. (7.5.8) we find similar behavior. Figure 7.11 shows plots of these $\dot{y}_0$ values for fixed $\dot{x}_0$. Plots for different values of $\dot{x}_0$ have similar features. Since the coordinates must evolve such that they remain on this Hamiltonian surface (also verified by the plots of the Hamiltonian such as Figure 7.10), we must conclude that as x_0 approaches zero, the $\dot{y}_0$ parameter must take on very large values. This in turn causes y_0 to take on large values which corresponds to a very sharp kink, much sharper than is physically reasonable. Therefore it appears that the ansatz in Eq. (7.2.3) is not sufficient to capture the observed behavior. Two possible deficiences of the ansatz are that it does not include any radiation degrees of freedom and that it

Figure 7.11: A two-dimensional Hamiltonian section for fixed $\dot{x}_0 = -0.9$.

does not include relativistic terms. Since the actual simulations showed that for small initial velocities very little energy was carried via emission of radiation, it would seem that the relativistic corrections are at the root of the problem. This is further supported by the fact that in all of the simulations of the ODEs, the velocities attained were relativistic. In addition we can look at the values of $\dot{x}_0$ allowed by the Hamiltonian. In Figure 7.12 we plot the Hamiltonian section for fixed $y_0 = 1$. Here we see that all of the velocities for x_0 near zero are indeed close to -1. What is even more striking is the fact that the velocity never exceeds -1, but turns around just before the limiting velocity is attained.

7.6 A "Relativistic" Ansatz

Since the original Lagrangian is Lorentz invariant, the boosted kink

$$\tanh\Big[\frac{m(x+x_0)}{\sqrt{2}\sqrt{1-\dot{x}_0^2}}\Big] \ , \tag{7.6.1}$$

is a solution to the equations of motion. This prompts one to modify the ansatz given in Eq. (7.2.3) to include the relativistic "γ" factor

$$\Phi_A(x,t) = \frac{m}{\sqrt{\lambda}}\Big\{1 - \tanh\Big[\frac{my_0\gamma(x-x_0)}{\sqrt{2}}\Big] + \tanh\Big[\frac{my_0\gamma(x+x_0)}{\sqrt{2}}\Big]\Big\} \ , \tag{7.6.2}$$

with γ given by

$$\gamma \equiv \frac{1}{\sqrt{1-\dot{x}_0^2}} \ . \tag{7.6.3}$$

By including the factor of γ we ensure that the width of the kink and antikink will decrease as the velocity increases. This may in fact take the place of the y_0 parameter, however we shall keep both coordinates initially to ensure the greatest flexibility.

Again we insert this ansatz into the expression for the Lagrangian density and integrate over space to obtain an effective Lagrangian

$$\begin{aligned} L(x_0,\dot{x}_0,\ddot{x}_0,y_0,\dot{y}_0) &= \gamma^2\left[\frac{1}{2}\tilde{m}_1(x_0,y_0)\dot{x}_0^2 + \tilde{m}_2(x_0,y_0)\dot{x}_0\dot{y}_0 + \frac{1}{2}\tilde{m}_3(x_0,y_0)\dot{y}_0^2\right] \\ + \quad & \frac{m^4\sqrt{2}}{2\lambda}\left\{\frac{4\gamma\dot{x}_0\ddot{x}_0}{m^3y_0^2}\Big[2\dot{y}_0 + \gamma^2y_0\dot{x}_0\ddot{x}_0\Big]w_3(z_0) + \frac{2\gamma^3x_0y_0\dot{x}_0^2\ddot{x}_0}{m}w_3(z_0)\right\} \\ - \quad & \gamma^2\tilde{V}_1(x_0,y_0) - \tilde{V}_2(x_0,y_0) \ , \end{aligned} \tag{7.6.4}$$

where

$$\tilde{m}_i \ \equiv m_i(x_0,\gamma y_0) \ , \tilde{V}_i \ \equiv V_i(x_0,\gamma y_0) \ , \tag{7.6.5}$$

Figure 7.12: A two dimensional Hamiltonian section for fixed $y_0 = 1$.

and the expressions for the functions $w_i(z_0)$ are given in Appendix I. Since this effective Lagrangian depends on the second time derivative of x_0, one must use second order variational methods [138, 139] to obtain the Euler-Lagrange equations of motions. Since the Lagrangian does not depend of the second time derivative of y_0, the standard Euler-Lagrange equation applies. The equation for x_0 is [140]

$$\frac{d^2}{dt^2}\frac{\partial L}{\partial \ddot{x}_0} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_0} + \frac{\partial L}{\partial x_0} = 0 \ . \tag{7.6.6}$$

Due to the additional terms in the Lagrangian and the equation of motion for x_0, the resulting set of coupled equations for x_0 and y_0 are extremely long and complex. Presently these equations are being derived and coded.

Although no results are yet available for the set of equations which result from carrying out the calculations in Eq. (7.6.6), the data in the previous sections indicates that a “relativistic” approach as outlined has some promise. The failure of the intuitive ansatz used in the previous sections indicates that either the relativistic corrections are needed or that a more sophisticated ansatz is required. Perhaps one needs to include the phonon degrees of freedom to achieve the quantitative agreement sought.

Chapter 8

Conclusions and Future Work

One of the most important results of this work is the formulation of a Newton's equation for the kink center of mass variable $X(t)$. The force which the kink experiences is found to depend on the phonons radiated by the interaction of the kink with the perturbation. The fact that these phonons appear in the kink center of mass equation demonstrates that the kink is an extended particle with internal degrees of freedom. This conclusion could be reached from purely numerical experiments in which the original PDE is solved "exactly". However the explicit separation of the degrees of freedom into kink and phonon components makes the analysis more physical. The first-order motion is especially easy to deduce since an effective potential exists for the kink center of mass variable. The second order motion is complicated by the appearance of the phonon degrees of freedom, but it is still tractable numerically. The specific applications of the perturbation theory presented here were chosen to mimic as closely as possible situations which might appear in real systems. One could easily imagine other perturbations which are less accurate approximations of the real situation (such as delta function potentials) for which the entire analysis (through second order) could be carried out analytically. This was illustrated when the thermal fluctuations were studied in Chapter 6. There we were able to derive a Fokker-Planck equation which again showed that the kink behaves, to lowest order, as a Newtonian particle.

One of the most interesting aspects of the present perturbation theory is the ability to describe shape changes of the kink waveform. In section 5.6 we saw that the ψ field accurately predicted the correct shape change for a kink which entered a new medium in which the limiting propagation speed was higher than the original medium. This shape change illustrates the fact that although the kink obeys Newtonian dynamics, it does not behave as a point particle; rather it behaves like an extended, deformable particle. The fact that the kink is an extended particle is not surprising, especially when one views the kink in the context of the pendulum chain. Here, we see that the kink is the result of a "cooperation" of many of the individual single pendulum degrees of freedom. The transformation which is the basis for our perturbation theory simply redistributes these degrees of freedom so that the kink may be described by only one coordinate.

In addition to describing kink shape changes, the ψ field must describe any phonons emitted and their influence on the kink motion. In section 5.3 we saw that one of the results of this interaction between the kink and phonon degrees of freedom is a transfer of energy from the kink to the phonons. This evidenced itself in a final kink velocity which was slightly lower than the initial velocity. In addition, we observed oscillations in the velocity about this final value, again indicative of a transfer of energy to and from other modes. One could imagine that similar energy transfer could occur when the kink-bearing system is coupled to different degrees of freedom. For example, in magnetic systems the kink represents a domain wall while the phonons represent spin waves. If the magneto-acoustic coupling constant is strong enough, one might find additional lattice vibrations induced when the kink collides with a magnetic impurity. This would possibly be observable as a contribution to the kink "viscosity".

Having gained some confidence with the method presented, we can look ahead to see other possible applications of the method. Due to the rather general form which the perturbation can take, many other relevant perturbations can be studied. It should be remembered that there are some interesting situations for which there is no perturbation present but in which the initial conditions are nontrivial. The simulations of Wada and Schrieffer [67] and Ogata and Wada [68] fall into this class, since they considered the collision of a prepared phonon packet with a stationary kink. To lowest order they find that the phonon packet is merely phase-shifted relative to the case in which no kink is present. To higher order they find the generation of reflected and transmitted phonons of frequency $2\omega_{\bar{q}}$ where $\bar{q}$ is the mean wave vector of the phonon packet. In addition the first and second order phase shifts experienced by the kink could be computed as a function of the mean frequency $\bar{q}$ and compared with the previous results. Through the use of the collective coordinate $X(t)$ one could hopefully come to a better understanding of the momentum transfer which occurs in these collisions.

Although the formal theory derived in Chapter 3 is set up to study time-dependent perturbations $v(x,t)$, our codes have not as yet been generalized to handle this situation. One of the interesting problems which could be studied with this capability is the damped, harmonically driven sine-Gordon equation. This particular equation has been the subject of several studies [28, 141, 142]. Although these simulations were carried out on the finite line, it would be interesting to see if the same types of chaos observed there arise in the infinite system. Since our ansatz includes only one kink and assumes that the phonon field ψ is small, the standard period-doubling route to chaos would evidence itself indirectly by the development of an instability. The instability would evidence itself by the developement of a phonon field which would try to produce another kink-like structure. Since this would require a rather large phonon field, this approach would only be able to indicate the onset of the period-doubled regime. The method presented by Tomboulis and Woo [46] may be better suited to study this system since it allows for more than one soliton component to be present. Even better suited to study this problem are the modulation equations derived by Erconali, McLaughlin and Forest [36] which are tailored to study the finite line with multiple solitons present. Currently Flesch and Forest are applying these equations to this problem. In particular they are trying to reproduce the behavior observed by Ariyasu and Bishop [143] in their simulations. In particular, Ariyasu and Bishop have observed an interesting hystersis in the damped driven sine-Gordon equation.

Another area which merits further study is our work involving the Fokker-Planck equation for the phase-space distribution function $P(X, p; t)$. In having derived the derivative transformation (see Appendix G) a major technical problem has been solved. It now remains to develop a convergent procedure which yields corrections to the first-order distribution functions already derived. In order to verify (or negate) the adiabatic assumption which allowed us to factor the phase-space distribution function into a product of a phonon and kink distribution function, the time dependence of solutions to the first-order Fokker-Planck equations must be investigated. Having resolved the question of equilbration times for the undriven system, a new steady state ansatz would be required to study the driven system. The resulting equations would allow us to calculate transport coefficients such as mobilities. One could attack the problem of transport from a more fundamental Boltzmann equation [144] approach. Once again the canonical nature of the transformation is of great benefit since the Jacobian of the transformation is unity.

Besides using the present theory to study additional applications, there is additional formal work to be done. As it stands, our theory is restricted to the study of low velocity kinks. Since the "Lorentz-boosted" solution

$$\phi_c\Big[\frac{x - vt}{\sqrt{1 - v^2}}\Big]$$

satisifies the unperturbed equation, one wonders if a canonical transformation is available which uses such a solution as a starting point. If such an approach fails, one might be able to make some progress using covariant collective coordinates [145, 146, 147].

A further relevant question involves the quantization of the system. One of the interesting problems to be attacked is soliton tunneling in the presence of pertubations. So far, however, only the statistical mechanics of the quantum system system has received attention [148, 149]. Tomboulis [45] approaches the problem semiclassically by promoting the variables to operators and the *Dirac* brackets to commutators, a procedure which is well defined because the transformation to the new variables is indeed canonical. A rather subtle point in carrying out this promotion involves using the correctly symmetrized form for the momentum operator Π_0. Once this promotion is completed one expands the ψ field in terms of normal-mode creation and annihilation operators. Transition matrix elements can then be calculated.

Gervais et al. [47] approach the quantization problem for the unperturbed system via a functional integral approach, writing the action in terms of the new variables. The point canonical transformation to the new variables in the action must be made carefully in order to be consistent [150]. When these points are taken care of, both the semiclassical and functional integral methods yield the same results to lowest order. Diagrammatic techniques based on the semiclassical approach [112] and functional integral [151] methods as applied to the perturbed problem are currently being investigated.

All of the quantum calculations mentioned above are carried out in the one soliton sector of the Fock space, that is to say, only one soliton is assumed to be present. Since many solitons can be present in a system, one really needs a formalism which can handle such instances. Of particular importance is the two-soliton case since the interaction between the solitons can greatly change the final state of the system as has been seen in the ϕ^4 kink-antikink collisions studied in Chapter 7. A rather natural approach would be to have creation and annihilation operators *for the solitons*. This approach has only been briefly studied by Mandelstam [152]. The collective-coordinate approach will undoubtedly be of value in these future investigations.

Appendix A

Equations of Motion via Euler-Lagrange Formalism

In this appendix we derive the equations of motion for the dynamical variables and from these we derive second-order equations for $X(t)$ and $\psi(x,t)$. As mentioned in Chapter 2, this involves taking the Dirac bracket of the dynamical variables with the Hamiltonian. To this end, the Hamiltonian was written as the sum of three terms, an unperturbed term H_0, an interaction term H_{int}, and H_{ψ_0} which involves terms proportional to the background field $\psi_0(x,t)$. The reason for writing H in this particular form is that Tomboulis [45] has already computed the Dirac bracket of the dynamical variables with the unperturbed contribution to the Hamiltonian. The results of these calculations are [45]

$$\{X, H_0\} = \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)^2} \; , \tag{A.1}$$

$$\{p, H_0\} = 0 \; , \tag{A.2}$$

$$\{\psi, H_0\} = \pi(x,t) + \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)^2}\left[\psi'(x,t) - \frac{1}{M_0}\xi\phi_c'(x)\right] , \tag{A.3}$$

$$\begin{aligned}\{\pi, H_0\} &= \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)^2}\left[\pi'(x,t) + \frac{1}{M_0}\phi_c'(x)\int \pi\phi_c'' - \frac{p + \int \pi\psi'}{M_0(1+\xi/M_0)}\phi_c''(x)\right] \\ &\quad +\psi''(x,t) - V'(\psi,\phi_c) + \frac{1}{M_0}\phi_c'(x)\left(\int \psi'\phi_c'' + \int V'\phi_c'\right) . \end{aligned} \tag{A.4}$$

Using the brackets given in Eqs. (3.3.10-11) one can calculate the following brackets

$$\{X, H_{\psi_0} + H_{int}\} = \frac{A(X,t)}{M_0(1+\xi/M_0)} \; , \tag{A.5}$$

$$\{p, H_{\psi_0} + H_{int}\} = -\int \pi'(x-X,t)\dot{\psi}_0(x,t) + \int \phi_c''(x-X)\psi_0'(x,t)$$

$$\begin{aligned}
&+ \quad \frac{p+\int \pi\psi}{M_0(1+\xi/M_0)}\int \phi_c''(x-X)\dot{\psi}_0(x,t) \\
&+ \quad \int \psi''(x,t)\psi_0'(x+X,t) + \\
&+ \quad \int U'[\Phi(x,t)][\phi_c'(x-X)+\psi(x-X,t)] \\
&+ \quad \frac{\partial}{\partial X}\int v(x,t)F[\Phi(x,t),\Phi_x(x,t)]\ , \qquad \text{(A.6)}
\end{aligned}$$

$$\begin{aligned}
\{\psi(x,t),H_{\psi_0}+H_{int}\} &= -\dot{\psi}_0(x+X,t)+\frac{\phi_c'(x)A}{M_0}+ \\
&\quad \frac{A}{M_0(1+\xi/M_0)}\Big[\psi'(x,t)-\frac{\xi\phi_c'(x)}{M_0}\Big]\ , \qquad \text{(A.7)} \\
\{\pi(x,t),H_{\psi_0}+H_{int}\} &= \Big(1-\mathcal{P}_{\phi_c}\Big)\Bigg\{\frac{A\pi'(x,t)}{M_0(1+\xi/M_0)}-\frac{A(p+\int\pi\psi')}{M_0(1+\xi/M_0)^2}\phi_c'' \\
+\psi_0''(x+X,t) &- (\Delta U)'+v(x+X,t)F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)] \\
&+ \frac{d}{dx}\Big[v(x+X,t)F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)]\Big]\Bigg\}\ , \qquad \text{(A.8)}
\end{aligned}$$

where

$$A(X,t)=\int \phi_c'(x-X)\dot{\psi}_0(x,t)\ , \qquad \text{(A.9)}$$

$$(\Delta U)'=\frac{\partial}{\partial\Phi}\Big(\Delta U[\Phi]\Big)\Big|_{\Phi=\Phi(x+X,t)}\ , \qquad \text{(A.10)}$$

and primes and dots denote derivatives with respect to the first and second arguments respectively (dots are not total time derivatives). Combining Eqs. (A1) to (A8) we can write

$$\begin{aligned}
\dot{X} &= \frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)^2}+\frac{A(X,t)}{M_0(1+\xi/M_0)}\ , \qquad \text{(A.11)} \\
\dot{p} &= \frac{\partial}{\partial X}\int v(x,t)F[\Phi,\Phi_x]-\int \pi'(x-X,t)\dot{\psi}_0(x,t) \\
&+ \frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)}\int\phi_c''(x-X)\dot{\psi}_0(x,t) \\
&+ \int\phi_c''(x-X,t)\psi_0(x',t)+\int\psi''(x-X)\psi_0'(x,t) \\
&+ \int U'[\Phi(x,t)]\Big(\phi_c'(x-X)+\psi(x-X,t)'\Big)\ , \qquad \text{(A.12)} \\
\dot{\psi}(x,t) &= \pi(x,t)+\frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)^2}\Big[\psi'(x,t)-\frac{\xi\phi_c'}{M_0}\Big]-\dot{\psi}_0(x+X,t) \\
&\quad +\frac{\phi_c'(x)A(X,t)}{M_0}+\frac{A(X,t)}{M_0(1+\xi/M_0)}\Big[\psi'(x,t)-\frac{\xi\phi_c'(x)}{M_0}\Big]\ , \qquad \text{(A.13)}
\end{aligned}$$

$$\begin{aligned}
\dot{\pi}(x,t) &= \Big(1-\mathcal{P}_{\phi_c}\Big)\Bigg\{\frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)^2}\Big[\pi'(x,t)-\phi_c''(x)\frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)}\Big] \\
&+ \psi''(x,t)-V'(\psi,\phi_c)+\frac{A\pi'(x,t)}{M_0(1+\xi/M_0)}-\frac{A(p+\int\pi\psi')}{M_0^2(1+\xi/M_0)^2}\phi_c'' \\
&+ \psi_0''(x+X,t)-(\Delta U)'+v(x+X,t)F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)] \\
&- \frac{d}{dx}\Big[v(x+X,t)F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)]\Big]\Bigg\}\ . \qquad \text{(A.14)}
\end{aligned}$$

Next we derive a second-order equation for the kink center of mass variable $X(t)$. We begin by taking a total time derivative of Eq. (A11) which may be written

$$\begin{aligned}
\ddot{X} = \frac{\dot{p}+\int\dot{\pi}\psi'+\int\pi\dot{\psi}'}{M_0(1+\xi/M_0)^2}-\frac{\int\phi_c'\dot{\psi}'}{M_0(1+\xi/M_0)}\dot{X} &- \frac{p+\int\pi\psi'}{M_0^2(1+\xi/M_0)^2}\int\phi_c'\dot{\psi}' \\
&+ \frac{1}{M_0(1+\xi/M_0)}\frac{d}{dt}A\ . \qquad \text{(A.15)}
\end{aligned}$$

We consider each of the terms in Eq. (A.15) in turn, first treating the $\int\dot{\pi}\psi'$ term. Using Eq. (A.14) for $\dot{\pi}$ and collecting terms we have

$$\begin{aligned}
\int\dot{\pi}\psi' &= \dot{X}\int\pi'\psi'+\frac{\dot{X}\xi}{M_0}\int\phi''\pi-\frac{(p+\int\psi'\pi)^2}{M_0(1+\xi/M_0)^3}\int\phi_c''\psi' \\
&- \int\Big[U'(\phi_c+\psi)-U'(\phi_c)\Big]\psi'+\frac{\xi}{M_0}\int\phi_c'[U'(\phi_c+\psi)-U'(\phi_c')] \\
&- \frac{A(p+\int\pi\psi')}{M_0^2(1+\xi/M_0)^2}\int\phi_c''\psi'+\int\psi_0''(x+X,t)\psi'-\frac{\xi}{M_0}\int\psi_0''(x+X,t)\phi_c' \\
&- \int\ (\Delta U)'\psi'+\frac{\xi}{M_0}\int\ (\Delta U)'\phi_c'+\frac{\xi}{M_0}\int\psi'\phi'' \\
&+ \int v(x,t)\psi'(x-X,t)F_{10}-\int\psi'(x-X,t)\frac{d}{dx}\Big(v(x,t)F_{01}\Big) \\
&- \frac{\xi}{M_0}\Big[\int v(x,t)\phi_c'(x-X,t)F_{10}-\int\phi_c'(x-X,t)\frac{d}{dx}\Big(v(x,t)F_{01}\Big)\Big]\ . \qquad \text{(A.16)}
\end{aligned}$$

Next we collect four of the terms in Eq. (A.16) together and write

$$\begin{aligned}
- \int\Big[U'(\phi_c+\psi)-U'(\phi_c)\Big]\psi'+\frac{\xi}{M_0}\int\phi_c'[U'(\phi_c+\psi)-U'(\phi_c)] \\
-\int\ (\Delta U)'\psi'+\frac{\xi}{M_0}\int\ (\Delta U)'\phi_c' = \\
(1+\frac{\xi}{M_0})\int U'[\Phi(x+X,t)]\phi_c'+\int\phi_c''\psi'+\int U'[\Phi(x,t)]\ \psi_0'(x+X,t)\ . \\
\text{(A.17)}
\end{aligned}$$

This allows us to write

$$\begin{aligned}
\int \dot{\pi}\psi' &= \dot{X}\int \pi'\psi' + \frac{\dot{X}\xi}{M_0}\int \phi_c''\pi - \frac{(p+\int\pi\psi')^2}{M_0(1+\xi/M_0)^3}\int \phi_c''\psi' \\
&+ (1+\frac{\xi}{M_0})\int U'[\Phi(x,t)]\phi_c'(x-X) + \int \phi_c''\psi' \\
&- \int U'[\Phi(x+X,t)][\phi_c'(x,t)+\psi'(x,t)] + \frac{\xi}{M_0}\int \psi'\phi_c'' \\
&- \frac{A(p+\int\pi\psi')}{M_0^2(1+\xi/M_0)^2}\int \phi_c''\psi' + \int \psi_0''(x+X,t)\psi' - \frac{\xi}{M_0}\int \psi_0''(x+X,t)\phi_c' \\
&+ \int v(x,t)\psi'(x-X,t)F_{10} - \int \psi'(x-X,t)\frac{d}{dx}\Big(v(x,t)F_{01}\Big) \\
&- \left[\frac{\xi}{M_0}\int v(x,t)\phi_c'(x-X,t)F_{10} - \int \phi_c'(x-X,t)\frac{d}{dx}\Big(v(x,t)F_{01}\Big)\right] \quad \text{(A.18)}
\end{aligned}$$

Next we we consider the $\int \pi\dot{\psi}'$ term for which we can write

$$\int \pi\dot{\psi}' = \dot{X}\int \pi\psi'' - \frac{\xi\dot{X}}{M_0}\int \pi\phi_c'' - \int \pi\dot{\psi}_0(x+X,t) + \frac{A}{M_0}\int \pi\phi_c'' \ . \quad \text{(A.19)}$$

Combining Eqs. (A.18) and (A.19) and using Eq. (A.12) for $\dot{p}$ we can write for the numerator of the first term of Eq. (A.15),

$$\begin{aligned}
\dot{p} + \int \dot{\pi}\psi' &+ \int \pi\dot{\psi}' = -\Big(1+\frac{\xi}{M_0}\Big)\int v(x,t)\Big[\phi_c'(x-X)F_{10} + \phi_c''(x-X)F_{01}\Big] \\
&+ \frac{p+\int\pi\psi'}{M_0(1+\xi/M_0)}\int \phi_c''(x-X)\dot{\psi}_0(x,t) \\
&+ (1+\frac{\xi}{M_0})\Bigg[(1-\dot{X}^2)\int \psi'\phi_c'' \\
&- \int \psi_0''(x,t)\phi_c'(x-X) + \int U'[\Phi(x,t)]\phi_c'(x-X)\Bigg] \\
&+ \frac{A(X,t)(p+\int\pi\psi')}{M_0^2(1+\xi/M_0)^2}\int \phi_c''\psi' + \frac{A^2(X,t)}{M_0^2(1+\xi/M_0)}\int \phi_c''\psi' \\
&+ \frac{A(X,t)}{M_0}\int \pi\phi_c'' \ . \quad \text{(A.20)}
\end{aligned}$$

Lastly, we compute $\int \phi_c'\dot{\psi}'$ and dA/dt:

$$\int \phi_c'\dot{\psi}' = \int \phi_c'\pi + \dot{X}\int \phi_c'\psi'' - \int \phi_c'\dot{\psi}_0'(x+X,t) \quad \text{(A.21)}$$

$$\frac{dA(X,t)}{dt} = \int \ddot{\psi}_0(x+X,t)\phi_c'(x) + \dot{X}\int \dot{\psi}_0'(x+X,t)\phi_c'(x) \ . \quad \text{(A.22)}$$

Combining Eqs. (A.20-22) we finally have

$$\begin{aligned}\ddot{X} &= \frac{1}{M_0(1+\xi/M_0)}\Big\{-\int v(x,t)\big[\phi_c'(x-X)F_{10}[\Phi(x,t),\Phi_x(x,t)] \\ &\qquad +\phi_c''(x-X)F_{01}[\Phi(x,t),\Phi_x(x,t)]\big] \\ &+ \int(\ddot{\psi}_0-\psi_0'')\phi_c'(x-X)+\int U'[\Phi(x,t)]\phi_c'(x-X)+(1+\dot{X}^2)\int\psi'\phi_c'' \\ &\qquad -2\dot{X}\int\pi'\phi_c'+2\dot{X}\int\phi_c'(x)\dot{\psi}_0'(x+X,t)\Big\}\ , \qquad \text{(A.23)}\end{aligned}$$

where we have repeatedly made use of Eq. (A.11). One can use the ψ_0 equation to replace the $\ddot{\psi}_0-\psi_0''$ term if desired.

In the same manner we could derive an exact second-order equation for $\psi(x,t)$. However, it would be extremely long and would not give us as much insight as the exact second-order equation for $X(t)$. Rather, we will derive a second-order differential equation for $\psi(x,t)$ which is valid to first-order in the perturbation strength. Taking the total time derivative of $\dot{\psi}$ given in Eq. (A.13) we have, keeping only terms of first-order in the perturbation,

$$\ddot{\psi}(x,t)=\dot{\pi}(x,t)-\ddot{\psi}_0(x+X,t)+\frac{\phi_c'(x)}{M_0}\frac{dA(X,t)}{dt}\ . \qquad \text{(A.24)}$$

Using expressions for $\dot{\pi}$ and dA/dt given by Eqs. (A.14) and (A.22) we have, again keeping only first-order terms in λ,

$$\begin{aligned}\ddot{\psi}(x,t) &= \psi''(x,t)-V'(\psi,\phi_c)-\frac{\phi_c'(x)}{M_0}\Big[\int\psi\phi_c''+\int V'(\psi,\phi_c)\phi_c\Big] \\ &+ (1-\mathcal{P}_{\phi_c})\Big\{\psi_0''(x+X,t)-(\Delta U)'+v(x+X,t)F_{10}[\Phi(x+X,t),\Phi_x(x+X,t)] \\ &- \frac{d}{dx}\Big(v(x+X,t)F_{01}[\Phi(x+X,t),\Phi_x(x+X,t)]\Big)-\ddot{\psi}_0(x+X,t)\Big\}\ . \qquad \text{(A.25)}\end{aligned}$$

Next we use the facts that

$$V'(\psi,\phi_c)=\psi(x,t)U''(\phi_c(x))+O(\lambda^2)\ , \qquad \text{(A.26)}$$

$$(\Delta U)'=\psi_0(x+X,t)U''(\phi_c)+O(\lambda^2)\ , \qquad \text{(A.27)}$$

and

$$\int\psi'\Big(\phi_c''+V'(\psi,\phi_c)\Big)=O(\lambda^2) \qquad \text{(A.28)}$$

to write

$$
\begin{aligned}
&\ddot{\psi}(x,t) - \psi''(x,t) + \psi(x,t)U''(\phi_c) = \\
&\quad (1-\mathcal{P}_{\phi_c})\Big\{ -\ddot{\psi}_0(x+X,t) + \psi_0''(x+X,t) - \psi_0(x+X,t)U''(\phi_c) \\
&\qquad\qquad + v(x+X,t)F_{10}[\Phi(x+X,t), \Phi_x(x+X,t)] \\
&\qquad\qquad - \frac{d}{dx}\Big(v(x+X,t)F_{01}[\Phi(x+X,t), \Phi_x(x+X,t)] \Big) \Big\} \; . \qquad \text{(A.29)}
\end{aligned}
$$

Finally we use the fact that ψ_0 satisifies Eq. (3.3.8) to obtain

$$
\begin{aligned}
&\ddot{\psi}(x,t) - \psi''(x,t) + \psi(x,t)U''(\phi_c) = \\
&\quad (1-\mathcal{P}_{\phi_c})\Big\{ \Big[1 - U''(\phi_c)\Big]\psi_0(x+X,t) + v(x+X,t)\Big[F_{10}[\phi_c, \phi_c'] - F_{10}[0,0]\Big] \\
&- \quad \frac{d}{dx}\Big[v(x+X,t)\Big(F_{01}[\phi_c, \phi_c'] - F_{01}[0,0] \Big) \Big] \Big\} \; . \qquad \text{(A.30)}
\end{aligned}
$$

Appendix B

Equations of Motion via Direct Substitution

In this appendix, we derive the equations of motion by simply substituting the kink variables for the original field variables in the equation of motion for the original fields. The Euler-Lagrange equation of motion for the original field $\Phi(x,t)$ can be derived from the Lagrangian density

$$\mathcal{L} = \frac{1}{2}\Phi_t^2 - \frac{1}{2}\Phi_x^2 - U(\Phi) + v(x,t)F[\Phi(x,t), \Phi_x(x,t)] \ . \tag{B.1}$$

We add to this equation of motion a phenomenological damping term of the form $\epsilon\dot{\Phi}(x,t)$ (when appropriate) thereby obtaining

$$\Phi_{tt} + \epsilon\Phi_t(x,t) - \Phi_{xx} + U'(\Phi) + \mathcal{G} = 0 \ . \tag{B.2}$$

where $\mathcal{G}$ is given by

$$\mathcal{G} = \frac{d}{dx}\Big[v(x,t)F_{01}[\Phi(x,t), \Phi_x(x,t)]\Big] - v(x,t)F_{10}[\Phi(x,t), \Phi_x(x,t)] \ . \tag{B.3}$$

Using as an ansatz for Φ

$$\Phi(x,t) = \phi_c[x - X(t)] + \psi[x - X(t), t] + \psi_0(x,t) \ , \tag{B.4}$$

we may compute the appropriate derivatives that occur in Eq. (B.2);

$$\begin{aligned}
\frac{d}{dt}\Phi(x,t) &= -\dot{X}\phi_c'[x - X(t)] - \dot{X}\psi'[x - X(t), t] + \dot{\psi}[x - X(t), t] \\
&+ \dot{\psi}_0(x,t) \ , \qquad \text{(B.5)} \\
\frac{d^2}{dt^2}\Phi(x,t) &= -\ddot{X}\Big\{\phi_c'[x - X(t)] + \psi'[x - X(t), t]\Big\} + \dot{X}^2\Big\{\phi_c''[x - X(t)]
\end{aligned}$$

$$
\begin{aligned}
& + \quad \psi''[x-X(t),t]\Big\} - 2\dot{X}\dot{\psi}'[x-X(t),t] \\
& + \quad \ddot{\psi}[x-X(t),t] + \ddot{\psi}_0(x,t) \ , \qquad \text{(B.6)}
\end{aligned}
$$

$$
\frac{d^2}{dx^2}\Phi(x,t) \ = \ \phi_c''[x-X(t)] + \psi''[x-X(t),t] + \psi_0''(x,t) \ , \qquad \text{(B.7)}
$$

where as before, primes and dots represent partial derivatives with respect to the first and second arguments respectively (a dot does not represent a total time derivative). To obtain an equation of motion for the center of mass coordinate $X(t)$, we substitute the expressions in Eqs. (B.5-7) into Eq. (B.2) , multiply by $\phi_c'[x-X(t)]$ and integrate over x. Using Eqs. (3.3.6-7) we have

$$
\begin{aligned}
[M_0+\xi]\ddot{X} \ &= \ \dot{X}^2\int\psi''\phi_c' - 2\dot{X}\int\dot{\psi}'\phi_c' + \int[\ddot{\psi}_0(x,t) - \psi_0''(x,t)]\phi_c'(x-X) \\
&- \ \int\psi''\phi_c' + \int U'[\Phi]\phi_c'(x-X) - \epsilon\dot{X}[M_0+\xi] \\
&+\epsilon\int\phi_c'(x-X)\dot{\psi}_0(x,t) + \int\phi_c'(x-X)\mathcal{G} \ , \qquad \text{(B.8)}
\end{aligned}
$$

where we have also used the fact that

$$
\int\ddot{\psi}\phi_c' = \int\dot{\psi}\phi_c' = 0 \ . \qquad \text{(B.9)}
$$

To put Eq. (B.8) into a form more easily compared with Eq. (A.23), we use Eq. (A.13) to substitute for $\dot{\psi}$, which after collecting like terms gives us

$$
\begin{aligned}
\ddot{X} \ = \ \frac{1}{M_0(1+\xi/M_0)}\Big\{ & -\int\phi_c'(x-X)\mathcal{G} + \int(\ddot{\psi}_0 - \psi_0'')\phi_c'(x-X) \\
& + \int U'[\Phi(x,t)]\phi_c'(x-X) + (1+\dot{X}^2)\int\psi'\phi_c'' \\
& -2\dot{X}\int\pi'\phi_c' + 2\dot{X}\int\phi_c'(x)\dot{\psi}_0'(x+X,t) \\
& +\epsilon\int\phi_c'(x-X)\dot{\psi}_0(x,t)\Big\} - \epsilon\dot{X} \ , \qquad \text{(B.10)}
\end{aligned}
$$

which agrees with Eq (A.23) for $\epsilon = 0$.

Similarly we can derive the ψ equation. To do this we merely write the full field equation in terms of the new variables which after rearrangement yields

$$
\begin{aligned}
& \ddot{\psi}[x-X(t),t] - \psi''[x-X(t),t] + U'[\Phi(x,t)] = \\
& \quad \ddot{X}\Big\{\phi_c'[x-X(t)] + \psi'[x-X(t)]\Big\} - \dot{X}^2\Big\{\phi_c''[x-X(t)] + \psi''[x+X(t),t]\Big\} \\
& + \ 2\dot{X}\dot{\psi}'[x-X(t),t] - \ddot{\psi}_0(x,t) + \phi_c''[x-X(t)] + \psi_0''(x,t) - \mathcal{G} \\
& - \ \epsilon\left[\dot{X}\Big(\phi_c'(x-X) + \psi'(x-X,t) + \dot{\psi}(x_X,t) + \psi_0(x_X,t)\Big)\right] . \qquad \text{(B.11)}
\end{aligned}
$$

Before we carry out a perturbation expansion of Eq. (B.10) we transform to a frame which moves with the kink. Since we don't know $X(t)$ exactly, we can transform to a frame $[y = x - X^{(1)}(t)]$ whose origin moves according to the first-order kink motion. In this frame, the kink velocity is of second-order in the perturbation and therefore we can neglect all terms in Eq. (B.11) which are proportional to $\dot{X}$ leaving us with

$$\begin{aligned}
\ddot{\psi}[y,t] &- \psi''[y,t] + U'[\phi_c(y,t)] + \Big(\psi(y,t) + \psi_0[y + X^{(1)}(t)]\Big)U''[\phi_c(y)] = \\
&- \left\{\frac{\phi_c'(y)}{M_0}\int \phi_c'[y - X^{(1)}(t)]\mathcal{G}\int(\ddot{\psi}_0 - \psi_0'')\phi_c'[y - X^{(1)}(t)]\right\} \\
&- \ddot{\psi}_0(y,t) + \phi_c''[y - X^{(1)}(t)] + \psi_0''(y,t) + \mathcal{G} \\
&- \epsilon\left[\dot{X}\Big(\phi_c'(x - X) + \psi'(x - X, t) + \dot{\psi}(x_X, t) + \psi_0(x_X, t)\Big)\right] \\
&+ \epsilon\frac{\phi_c'(y)}{M_0}\int \phi_c'(x - x)\dot{\psi}_0(x,t) \ . \qquad \text{(B.12)}
\end{aligned}$$

Cancelling common terms and using the projection operator notation we have

$$\begin{aligned}
\ddot{\psi}[y,t] &- \psi''[y,t] + \psi(y,t)U''[\phi_c(y)] \\
&= \Big(1 - \mathcal{P}_{\phi_c}\Big)\Big\{-\mathcal{G} - \ddot{\psi}_0 + \psi_0'' - \psi_0[y + X^{(1)}(t)]U''[\phi_c(x)] \\
&- \epsilon\dot{\psi} + \dot{\psi}_0(y + X^{(1)})\Big\} \ . \qquad \text{(B.13)}
\end{aligned}$$

Finally using Eq. (3.3.8) to first-order in the perturbation strength, we have

$$\begin{aligned}
&\ddot{\psi}[y,t] - \psi''[y,t] + \psi(y,t)U''[\phi_c(y)] = \\
&\qquad \Big(1 - \mathcal{P}_{\phi_c}\Big)\Big\{\psi_0[y + X^{(1)}(t)]U''[\phi_c(x)] \\
&+ \ v[y + X^{(1)}(t)]\Big(F_{10}[\phi_c(y)], \phi_c'(y)] - F_{10}[0,0]\Big) \\
&- \ v'[y + X^{(1)}(t)]\Big(F_{01}[\phi_c(y)], \phi_c'(y)] - F_{01}[0,0]\Big) \\
&- \ v[y + X^{(1)}(t)]\Big(\phi_c'(y)F_{11}[\phi_c(y)], \phi_c'(y)] - \phi_c''(y)F_{02}[\phi_c(y)], \phi_c'(y)]\Big) \\
&- \ \epsilon\dot{\psi} + \dot{\psi}_0(y + X^{(1)})\Big\} \ , \qquad \text{(B.14)}
\end{aligned}$$

which is equivalent to what is given in Eq. (A.30).

Appendix C

Evaluation of the integral $J(\beta^2)$

The integral $J(\beta^2)$ [Eq. (4.1.50)] differs from Hardy's integral for Lommel functions [91, 92] only in that in the denominator, t^2+1 is replaced by $t^2+\beta^2$. The only restriction placed on β is that $\Re(\beta) > 0$. We first consider the case in which $b < 0$ for which we have from the tables [153],

$$J(\beta^2) = \frac{1}{\pi}\int_0^\infty \frac{t\ dt}{t^2+\beta^2}\sin\Big[at + \frac{b}{t}\Big] = \frac{1}{2}e^{-(a\beta_- - \frac{b}{\beta_-})}\ , \tag{C.1}$$

where the restriction $\Re(b) > 0$ is required.

For $b > 0$ we distinguish between $b < a$ and $b > a$. The latter may be reduced to the $b < a$ case by using the relation [154],

$$\frac{1}{\pi}\int_0^\infty \frac{t\ dt}{t^2+\beta^2}\sin\Big[at + \frac{b}{t}\Big] = J_0(2\sqrt{ab}) - \frac{1}{\pi}\int_0^\infty \frac{t\ dt}{t^2+\frac{1}{\beta^2}}\sin\Big[\frac{a}{t} + bt\Big]\ . \tag{C.2}$$

Therefore we need only consider $b < a$. Without loss of generality we may confine our attention to $|\beta| = 1$ by writing $\beta = |\beta|e^{i\varphi}$ which allows us to write

$$\begin{aligned} J(\beta^2) &= \frac{1}{\pi}\int_0^\infty \frac{t\ dt}{|\beta|^2[\frac{t^2}{|\beta|^2}+e^{2i\varphi}]}\sin\Big[at + \frac{b}{t}\Big]\ , & \text{(C.3)}\\ &= \frac{1}{\pi}\int_0^\infty \frac{t\ dt}{t^2+e^{2i\varphi}}\sin\Big[a't + \frac{b'}{t}\Big]\ , & \text{(C.4)}\end{aligned}$$

where a' and b' are a and b scaled by $1/|\beta|$. Therefore, with $b < a$ and $|\beta| = 1$, we define

$$x \equiv 2\sqrt{ab} \quad , \quad c \equiv \frac{1}{\beta}\sqrt{\frac{a}{b}}\ , \tag{C.5}$$

in terms of which we may write $J(\beta^2)$ as

$$
\begin{aligned}
J(\beta^2) &= \frac{1}{\pi}\int_0^\infty \frac{t\ dt}{t^2+\beta^2}\sin\Big[\frac{x}{2}\Big(t\sqrt{\frac{a}{b}}+\frac{1}{t}\sqrt{\frac{b}{a}}\Big)\Big]\ , &\text{(C.6)}\\
&= \frac{c}{\pi}\int_{-\infty}^\infty \frac{e^u du}{ce^u+\frac{1}{ce^u}}\sin[x\cosh(u)]\ , &\text{(C.7)}\\
&= \frac{c}{\pi}\int_0^\infty du\Big\{\frac{e^{-u}}{ce^{-u}+(ce^{-u})^{-1}}+\frac{e^u}{ce^u+(ce^u)^{-1}}\Big\}\sin[x\cosh(u)]\ , &\text{(C.8)}\\
&= \frac{1}{2\pi}\int_1^\infty \frac{d\tau}{\sqrt{\tau^2-1}}\frac{c^2-1+2\tau^2}{\theta^2+\tau^2}\sin(x\tau)\ , &\text{(C.9)}
\end{aligned}
$$

with

$$\theta \equiv \frac{1}{2}(c-\frac{1}{c}) = \frac{c'^2+1}{2c'}\Big\{\frac{c'^2-1}{c'^2+1}\Re(\beta)-i\Im(\beta)\Big\}\ , \quad \text{(C.10)}$$

$$c' \equiv \sqrt{\frac{b}{a}}\ . \quad \text{(C.11)}$$

Since $\Re(b) > 0$ and $c' < 1$, θ is never pure imaginary, therefore θ^2 does not lie on the negative real axis and the only poles of the integrand in Eq. (C.9) are at $\tau = \pm 1$. We evaluate Eq. (C.9) by considering the contour integral $\Gamma(\beta^2)$ given by

$$\Gamma(\beta^2) \equiv \int_\Gamma \frac{dz\ e^{ixz}}{\sqrt{z^2-1}}\frac{c^2-1+2z^2}{\theta^2+z^2}\ . \quad \text{(C.12)}$$

With the branch cuts chosen as in Figure C.1, $\Gamma(\beta^2)$ becomes

$$\Gamma(\beta^2) = 2i\int_1^\infty \frac{d\tau\sin(x\tau)}{\sqrt{\tau^2-1}}\frac{c^2-1+2\tau^2}{\theta^2+\tau^2} - 2i\int_{-1}^1 \frac{d\tau\ e^{(ix\tau)}}{\sqrt{1-\tau^2}}\frac{c^2-1+2\tau^2}{\theta^2+\tau^2}\ , \quad \text{(C.13)}$$

therefore we have for $J(\beta^2)$,

$$
\begin{aligned}
J(\beta_-^2) &= \frac{1}{2\pi i}\frac{\Gamma(\beta^2)}{2}+\frac{1}{2\pi}\int_0^1 \frac{d\tau\cos(x\tau)}{\sqrt{1-\tau^2}}\frac{c^2-1+2\tau^2}{\theta^2+z^2}\ , &\text{(C.14)}\\
&= \frac{Res[f(z);-i\theta]}{2}+\frac{1}{2\pi}\int_0^{\frac{\pi}{2}} d\varphi\ \cos[x\cos(\varphi)]\frac{c^2-1+2\cos^2(\varphi)}{\theta^2+\cos^2(\varphi)}\ , &\text{(C.15)}
\end{aligned}
$$

where $Res[f(z);-i\theta]$ is the residue of $f(z)$ evaluated at $-i\theta$ with $f(z)$ given by the integrand of Eq. (C.12). In writing Eq. (C.14) we have used the fact the

Figure C.1: Contour for the integral $\Gamma(\beta^2)$

contributions to $\Gamma(\beta^2)$ from the large and small semicircles vanish when $R \to \infty$ and $\delta \to\ 0$ respectively. Evaluating the residue at the simple pole $-i\theta$ we have

$$Res[f(z); -i\theta] = e^{-(a\beta - \frac{b}{\beta})} \ . \tag{C.16}$$

The remaining integral in Eq. (C.15) may be evaluated by noting that

$$\frac{c^2 - 1 + 2\cos^2(\varphi)}{\theta^2 + \cos^2(\varphi)} = -4\sum_{k=1}^{\infty}(ic)^{2k}\cos(2k\varphi) \ . \tag{C.17}$$

Since $c < 1$, the sum in Eq. (C.17) is uniformly convergent and we may insert it into Eq. (C.15) and integrate term by term. We also make the substitution

$$\cos[x\cos(\varphi)] = J_0(x) + 2\sum_{n=1}^{\infty}(-1)^n J_{2n}(x)\cos(2n\varphi) \ , \tag{C.18}$$

The double sum resulting from substitution of Eqs. (C.17) and (C.18) into (C.15) is reduced to a single sum by orthogonality of $\cos(2n\varphi)$ on $[0, \frac{\pi}{2}]$, leaving us with

$$\frac{1}{2\pi}\int_0^{\infty}\frac{d\tau\cos(x\tau)}{\sqrt{1-\tau^2}}\frac{c^2 - 1 + 2\tau^2}{\theta^2 + z^2} = -\sum_{k=1}^{\infty}c^{2k}J_{2k}(x) \ , \tag{C.19}$$

$$= -\Lambda_2\Big[\frac{2b}{\beta}, 2\sqrt{ab}\Big] \ . \tag{C.20}$$

Finally collecting Eqs. (C.1), (C.16) and (C.20) we have

$$J(\beta^2) = \frac{1}{2} e^{-(a\beta - \frac{b}{\beta})} - \theta(b)\Lambda_2\Big[\frac{2b}{\beta}, \sqrt{2ab}\Big] \; , \tag{C.21}$$

where $\theta(b)$ is the Heaviside step function.

Appendix D

Lommel Functions of Two Variables

In Chapter 4 we obtained analytic expressions for several Green functions in terms of "modified" Lommel functions of two variables (not to be confused with Lommel functions of one variable $s_{\mu,\nu}(z)$ or $S_{\mu,\nu}(z)$). Since these functions are somewhat obscure, we shall review some of the existing literature which illustrates properties of Lommel functions and numerical techniques which have been applied to evaluate the functions. We end this appendix with the derivation of some properties of the modified functions which were useful in the derivation of the Green functions in Chapter 4.

Lommel functions were first studied by Lommel in his studies of diffraction at a straight edge [155] and a circular aperature [156]. In these works, Lommel gives a detailed discussion of what have become known as Lommel functions of two variables $U_n(w,s)$ and $V_n(w,s)$, which are defined by the series

$$U_n(w,s) = \sum_{m=0}^{\infty} (-1)^m \Big(\frac{w}{s}\Big)^{2m+n} J_{2m+n}(s) \ , \tag{D.1}$$

$$V_n(w,s) = \sum_{m=0}^{\infty} (-1)^m \Big(\frac{w}{s}\Big)^{-(2m+n)} J_{-(2m+n)}(s) \ . \tag{D.2}$$

Among the properties examined are recurrence relations, integral expressions and values for special arguments. He also gives some short tables and plots for real values of w and s. Many of these results are reproduced in Appendix II of Walker's *The Analytical Theory of Light* [157] as well as in Watson [91]. Lommel functions continue to be of use in the study of the propagation of electromagnetic radiation in a variety of media [158, 159, 160, 161].

Although Lommel functions of two variables have not received a great deal of attention since Lommel's original publications, several new properties and/or relations have been discovered. In particular, Shastri [162] presents some integral transforms related to the Laplace transform of the Lommel functions along with integrals of Lommel functions multiplied by Bessel functions, Fresnel functions, sines and cosines (these are not Fourier transforms due to the scaled arguments used) and other Lommel functions. Dekanosidze [163] shows that the functions $U_n(\xi, \eta)$ are solutions of the hyperbolic equation

$$\frac{\partial^2 U}{\partial\xi\partial\eta} + U = 0 \ , \tag{D.3}$$

with $\xi = s^2/2w$ and $\eta = w/2$. In addition, he derives about 15 complicated relations between the functions, one of the simpler being

$$U_\nu(w, s) = U_\nu(s^2/w, s) + \frac{1}{2} \int_{s^2/w}^{w} dx \ J_{\nu-1}(x) J_0\Big[\sqrt{\big(x - s^2/w\big)(x - w)}\Big] \ . \tag{D.4}$$

Several of these relations may prove useful when the functions are actually evaluated numerically.

The first numerical evaluation of the functions was carried out by Lommel himself in 1886. A more comprehensive table was published by Dekanosidze [164] in 1956, again for only real values of w and s. Additional studies for real values have been carried out by Rayleigh [165], Hopkins [166], Conrady [167], Buxton [168], Boersma [169] and Rybner [170]. The functions of purely imaginary argument, denoted by

$$Y_n(w, s) \equiv i^{-n} U_n(iw, is) = \sum_{m=0}^{\infty} \big(\frac{w}{s}\big)^{2m+n} I_{2m+n}(s) \ , \tag{D.5}$$

$$\Theta_n(w, s) \equiv i^{-n} V_n(iw, is) = \sum_{m=0}^{\infty} \big(\frac{w}{s}\big)^{-(2m+n)} I_{-(2m+n)}(s) \ , \tag{D.6}$$

have been tabulated by Kuznetsov [171] and Bark and Kuznetsov [172]. To our knowledge, no one has studied the "modified" functions which we define to be

$$\Lambda_n(w, s) \ \equiv \ i^{-n} U_n(iw, s) = \sum_{m=0}^{\infty} \Big(\frac{w}{s}\Big)^{2m+n} J_{2m+n}(s) \ , \tag{D.7}$$

$$\Xi_n(w, s) \ \equiv \ i^{-n} V_n(iw, s) = \sum_{m=0}^{\infty} \Big(\frac{w}{s}\Big)^{-2m-n} J_{-2m-n}(s) \ . \tag{D.8}$$

The numerical evaluation of the modified functions is presented in Appendix E along with a new asymptotic expansion. The treatment in Appendix E applies to complex values of w so the formula therein may be used to calculate Lommel functions of two real variables.

Now we turn our attention to deriving a few properties of the Lommel functions for the special case in which the arguments are of the form

$$\begin{aligned} w &= \beta(\tau - |z|) \ , \\ s &= \sqrt{\tau^2 - z^2} \ , \end{aligned} \tag{D.9}$$

with β a complex constant independent of τ and z. We restrict ourselves to the $U_n(w,s)$ Lommel functions although similar relations exist for the $V_n(w,s)$ functions and may be found in the literature [91, 162, 163]. Using the recurrence relation for Bessel functions [173], and the defining series of Lommel functions,

$$U_n(w,s) = \sum_{m=0}^{\infty} (-1)^{2m+n} J_{2m+n}(s) \ , \tag{D.10}$$

one may derive the following:

$$U_n(w,s) = \left(\frac{w}{s}\right)^n J_n(s) - U_{n+2}(w,s) \ , \tag{D.11}$$

$$\frac{\partial U_n(w,s)}{\partial s} = -\frac{s}{w} U_{n+1}(w,s) \ , \tag{D.12}$$

$$\frac{\partial U_n(w,s)}{\partial w} = \frac{1}{2} U_{n-1}(w,s) + \frac{1}{2}\left(\frac{s}{w}\right)^2 U_{n+1}(w,s) \ . \tag{D.13}$$

For the variables (w,s) as defined in Eq. (D.9) we have

$$\frac{\partial U_n(\beta w,s)}{\partial |z|} = -\frac{1}{2}\Big[\beta U_{n-1}(\beta w,s) + \frac{1}{\beta} U_{n+1}(\beta w,s)\Big] \ , \tag{D.14}$$

$$\frac{\partial U_n(\beta w,s)}{\partial \tau} = -\frac{1}{2}\Big[\beta U_{n-1}(\beta w,s) - \frac{1}{\beta} U_{n+1}(\beta w,s)\Big] \ , \tag{D.15}$$

$$\frac{\partial^2 U_n(\beta w,s)}{\partial^2 |z|^2} = \frac{1}{4}\Big[\beta^2 U_{n-2}(\beta w,s) + 2U_n(\beta w,s) + \frac{1}{\beta^2} U_{n+2}(\beta w,s)\Big] \ , \tag{D.16}$$

$$\frac{\partial^2 U_n(\beta w,s)}{\partial^2 \tau^2} = \frac{1}{4}\Big[\beta^2 U_{n-2}(\beta w,s) - 2U_n(\beta w,s) + \frac{1}{\beta^2} U_{n+2}(\beta w,s)\Big] \ , \tag{D.17}$$

Subtracting Eq. (D.16) from Eq. (D.17) we have

$$\frac{\partial^2 U_n(\beta w,s)}{\partial^2 \tau^2} - \frac{\partial^2 U_n(\beta w,s)}{\partial^2 |z|^2} = -U_n(\beta w,s) \ . \tag{D.18}$$

Therefore $U_n(\beta w,s)$ is a solution of the "massive" Klein-Gordon equation (at least in the positive half-space since $|z| > 0$).

The above properties hold for arbitrary complex w and s. We now focus on the modified functions in which w is pure imaginary. Introducing the notation

$$\Lambda_n(w,s) = i^{-n} U_n(iw,s) \ , \tag{D.19}$$

with w and s given by Eq. (D.9), we consider the limit in which $z \to 0$ for which

$$\frac{w}{s} = \sqrt{\frac{\tau - |z|}{\tau + |z|}} \to 1 \ . \tag{D.20}$$

For n even we have

$$\Lambda_{2n}(\tau,\tau) = -\sum_{m=1}^{n-1} J_{2m}(\tau) + \frac{1 - J_0(\tau)}{2} \ . \tag{D.21}$$

For odd n we use an integral representation

$$\Lambda_{2n+1}(\tau,\tau) = -\sum_{m=0}^{n-1} J_{2m+1}(\tau) + \frac{1}{2}\int_0^{\infty} dx J_0(x) \ , \tag{D.22}$$

or in terms of Struve functions [174],

$$\Lambda_{2n+1}(\tau,\tau) = -\sum_{m=0}^{n-1} J_{2m+1}(\tau) + \frac{1}{2}\Big\{\tau J_0(\tau) + \frac{\pi\tau}{2}[J_1(\tau)\mathbf{H}_0(\tau) - J_0(\tau)\mathbf{H}_1(\tau)]\Big\} \ . \tag{D.23}$$

Finally we consider the limiting case of $\tau = |z|$, i.e. $s = w = 0$. Since for all $n \geq 1$ $J_n(0) = 0$, we have

$$\begin{aligned} \Lambda_0(0,0) &= 1 \ , \\ \Lambda_n(0,0) &= 0 \quad n \geq 1 \ . \end{aligned} \tag{D.24}$$

While some of the properties (especially D.18) derived above are useful for the actual derivation of the Green functions in Chapter 4, they are most useful when checking the analytic expressions by operating on them with the differential operator

$$\partial_{tt} - \partial_{xx} + U''[\phi_c(x)] \ . \tag{D.25}$$

Appendix E

Numerical Evaluation and Asymptotic Forms of Modified Lommel Functions of Two Variables

Numerical evaluation of the Green functions derived in Chapter 4 requires an evaluation of the modified Lommel functions. Although Lommel functions of two real variables [164] and two purely imaginary variables [172] have been studied, to our knowledge no one has yet considered the modified functions. Below we present methods which are valid for w complex and s real (since we start by considering the modified functions and w may be complex, our methods also include the case of two real variables). Representing the first argument as βw, where $|\beta| = 1$ and w and s are real, we have for the defining series

$$\Lambda_n\left(\beta w, s\right) = \sum_{m=0}^{\infty} \left(\frac{\beta w}{s}\right)^{2m+n} J_{2m+n}\left(s\right) \ , \tag{E.1}$$

from which we deduce the symmetries

$$\begin{aligned} \Lambda_n(-\beta w, s) &= (-1)^n \Lambda_n(\beta w, s) \ , \\ \Lambda_n(\beta w, -s) &= \Lambda_n(\beta w, s) \ . \end{aligned} \tag{E.2}$$

From Eqs. (E.2) we see that we need only investigate the first quadrant of the w–s plane. Another relationship exists which allows us to further restrict our attention to the angular region $(0, \pi/4)$, i.e. the first octant. We obtain this property by recalling the generating function for Bessel functions [175]:

$$e^{\frac{s}{2}[\beta\kappa - \frac{1}{\beta\kappa}]} = \sum_{m=-\infty}^{\infty} (\beta\kappa)^m J_m(s) \ , \tag{E.3}$$

where $\kappa \equiv w/s$. Using the symmetry of the Bessel functions about the origin we have,

$$\begin{aligned}
\sinh\Big[\frac{s}{2}\Big(\beta\kappa - \frac{1}{\beta\kappa}\Big)\Big] &= \sum_{m=-\infty}^{\infty} (\beta\kappa)^{2m} J_{2m}(s) \ , \\
\cosh\Big[\frac{s}{2}\Big(\beta\kappa - \frac{1}{\beta\kappa}\Big)\Big] &= \sum_{m=-\infty}^{\infty} (\beta\kappa)^{2m+1} J_{2m+1}(s) \ .
\end{aligned} \tag{E.4}$$

Next we note that

$$\Lambda_n\Big(\frac{s^2}{\beta w}, s\Big) = \sum_{m=0}^{\infty} \Big(\frac{s}{\beta w}\Big)^{2m+n} J_{2m+n}(s) \ , \tag{E.5}$$

which leads us to

$$\begin{aligned}
\sinh\Big[\frac{s}{2}\Big(\beta\kappa - \frac{1}{\beta\kappa}\Big)\Big] &= \Lambda_1(\beta w, s) - \Lambda_1\Big(\frac{s^2}{\beta w}, s\Big) \ , \\
\cosh\Big[\frac{s}{2}\Big(\beta\kappa - \frac{1}{\beta\kappa}\Big)\Big] &= J_0(s) + \Lambda_0(\beta w, s) + \Lambda_0\Big(\frac{s^2}{\beta w}, s\Big) \ .
\end{aligned} \tag{E.6}$$

From Eqs. (E.6) we see that we have a relationship which allows us to consider only the region of the first quadrant of the s–w plane in which $w/s < 1$, namely the first octant. In this region the series definition (E.1) converges uniformly, however that rate of convergence is very slow when one approaches $w/s = 1$. By comparison with the geometric series we see that since $J_n(s) < 1 \ \forall \ n$, we have as an error estimate for truncation after N terms

$$R_N < \frac{\kappa^{2N}}{1-\kappa^2} \ , \tag{E.7}$$

We note that the error estimate in Eq. (E.7) is very crude as it does not take into account the decaying nature of the Bessel functions, however it suffices for our calculations.

As $w/s \to 1$, the number of terms in the series needed to attain a given accuracy becomes unreasonably large. For values of $\kappa = w/s$ larger than some κ_0, we turn to an asymptotic expansion [176] of the modified Lommel functions. We begin by following Mayall's [177] procedure for obtaining an integral representation for the Lommel functions by substitution of an integral representation for the Bessel functions into the series and summing the series explicitly. We restrict ourselves to deriving expressions for Λ_0 and Λ_1. For small n the asymptotic expansion for Λ_n may be obtained from the recurrence relation for Lommel functions. The large n limit has not yet been examined.

Starting with the integral representation for Bessel functions

$$J_{2m}(s) = \frac{(-1)^m}{\pi} \int_0^\pi d\theta e^{is\cos(\theta)} \cos(2m\theta) \ , \tag{E.8}$$

we have

$$\begin{aligned}
\Lambda_0(\beta w, s) &= \sum_{m=0}^{\infty} (\beta\kappa)^{2m} (-1)^m \frac{1}{\pi} \int_0^\pi d\theta e^{is\cos(\theta)} \cos(2m\theta) \ , && \text{(E.9)} \\
&= \frac{1}{\pi} \int_0^\pi d\theta \frac{1 + (\beta\kappa)^2 \cos(2\theta)}{1 + 2(\beta\kappa)^2 \cos(2\theta) + (\beta\kappa)^4} e^{is\cos(\theta)} \ , && \text{(E.10)} \\
&= \frac{J_0(s)}{2} + \frac{1 - (\beta\kappa)^4}{2\pi} \int_0^\pi d\theta \frac{e^{is\cos(\theta)}}{1 + 2(\beta\kappa)^2 \cos(2\theta) + (\beta\kappa)^4} \ , && \text{(E.11)} \\
&= \frac{J_0(s)}{2} + \sigma_1(\beta,\kappa) \frac{\epsilon(\beta,\kappa)}{\pi} \int_0^\pi d\theta \frac{e^{is\cos(\theta)}}{\epsilon^2(\beta,\kappa) + \cos^2(\theta)} \ , && \text{(E.12)}
\end{aligned}$$

where

$$\begin{aligned}
\epsilon(\beta,\kappa) &\equiv \frac{1 - (\beta\kappa)^2}{2\beta\kappa} \ , \\
\sigma_1(\beta,\kappa) &\equiv \frac{1 + (\beta\kappa)^2}{4\beta\kappa} \ , && \text{(E.13)}
\end{aligned}$$

and uniform convergence of the sum has been used. Similarly we may write

$$\Lambda_1(\beta w, s) = -\sigma_2(\beta,\kappa) \frac{d}{ds} \frac{\epsilon(\beta,\kappa)}{\pi} \int_0^\pi d\theta \frac{e^{is\cos(\theta)}}{\epsilon^2(\beta,\kappa) + \cos^2(\theta)} \ , \tag{E.14}$$

with

$$\sigma_2(\beta,\kappa) \equiv \frac{1 + (\beta\kappa)^2}{4} + \frac{\beta\kappa[1 + \epsilon^2(\beta,\kappa)]}{2\epsilon(\beta,\kappa)} \ . \tag{E.15}$$

At this point, Mayall's method no longer applies (unless $\beta = \pm i$) and we turn to an alternate derivation.

The integral $I(\epsilon, s)$ given by

$$I(\epsilon, s) = \frac{\epsilon}{\pi} \int_0^\pi d\theta \frac{e^{is\cos(\theta)}}{\epsilon^2 + \cos^2(\theta)} \ , \tag{E.16}$$

which occurs in Eqs. (E.12) and (E.14), is strong function of ϵ since in the limit as $\epsilon \to 0$ ($w/s \to 1$), we obtain a delta function. Other major contributions occur

Figure E.1: Contour for the asymptotic values of the Lommel functions.

at the stationary points $\theta = 0, \pi$. To evaluate $I(\epsilon, s)$, we substitute $t = \cos(\theta)$, deform the contour and represent the integrals as a residue which captures the strong ϵ behavior, plus two integrals for which asymptotic expansions are easily derived. Substituting we have

$$I(\epsilon, s) = \frac{\epsilon}{\pi} \int_{-1}^{1} d\theta \frac{e^{ist}}{(\epsilon^2 + t^2)\sqrt{1 - t^2}} , \tag{E.17}$$

$$= \frac{\epsilon}{\pi} \left\{ 2\pi i Res[f(z), i\epsilon] - \int_{c_1} dz \frac{e^{isz}}{(\epsilon^2 + z^2)\sqrt{1 - z^2}} - \int_{c_3} dz \frac{e^{isz}}{(\epsilon^2 + z^2)\sqrt{1 - z^2}} \right\} , \tag{E.18}$$

where $f(z)$ is given by

$$f(z) = \frac{\epsilon}{\pi} \frac{e^{isz}}{(\epsilon^2 + z^2)\sqrt{1 - z^2}} , \tag{E.19}$$

and the contours are shown in Figure E.1. We have used the fact that as $\delta \to 0$ and $y_0 \to \infty$, the contributions from the contours $c_{\delta 1}$, $c_{\delta 2}$ and c_2 vanish by Jordan's lemma. Evaluating the residue and shifting the variables, we have

$$\begin{aligned} I(\epsilon, s) &= \frac{e^{-\epsilon s}}{\sqrt{1+\epsilon^2}} - \int_0^{i\infty} dz \frac{e^{isz}e^{is}}{[\epsilon^2 + (z+1)^2]\sqrt{1-(z+1)^2}} \\ &- \int_{i\infty}^0 dz \frac{e^{isz}e^{-is}}{[\epsilon^2 + (z-1)^2)]\sqrt{1-(z-1)^2}} \ , \qquad \text{(E.20)} \\ &= \frac{e^{-\epsilon s}}{\sqrt{1+\epsilon^2}} - \frac{\epsilon}{\pi}[J + J^*] \ , \qquad \text{(E.21)} \end{aligned}$$

where

$$\begin{aligned} J &\equiv ie^{is}\int_0^\infty dy \frac{e^{-sy}}{[\epsilon^2 + (iy+1)^2]\sqrt{1-(iy+1)^2}} \ , \qquad \text{(E.22)} \\ &= 2ie^{is}\int_0^\infty dx \frac{e^{-sx^2}}{[\epsilon^2 + (ix^2+1)^2)\sqrt{x^2-2i}} \ , \qquad \text{(E.23)} \end{aligned}$$

As written in Eq. (E.23), J is in one of Dingle's [178] standard integral forms which has as an asymptotic expansion

$$J \approx 2ie^{is}\sqrt{\frac{\pi}{2F_{01}}}e^{-F_0}\sum_{n=0}^{\infty} Q_r \ , \qquad \text{(E.24)}$$

where

$$\begin{aligned} Q_0 &= G_0 \ , \\ Q_1 &= \frac{-\sqrt{2}}{3\sqrt{\pi}F_2^{\frac{3}{2}}}[-3G_1F_2] \ , \\ Q_2 &= \frac{1}{24F_2^3}[12G_2F_2^2] \ , \\ Q_3 &= \frac{-\sqrt{2}}{135\sqrt{\pi}F_2^{\frac{9}{2}}}[-45G_4F_2^4] \ , \\ Q_4 &= \frac{1}{1152F_2^6}[144G_4F_2^4] \ , \qquad \text{(E.25)} \\ F_\nu &= \left(\frac{d}{dx}\right)^\nu sx^2 \ , \qquad \text{(E.26)} \\ G_\nu &= \left(\frac{d}{dx}\right)^\nu \frac{1}{[\epsilon^2 + (ix^2+1)^2]\sqrt{x^2-2i}} \ . \qquad \text{(E.27)} \end{aligned}$$

Carrying out the derivatives, we have, including up to Q_4

$$J + J^* = -\frac{2}{1+\epsilon^2}\sqrt{\frac{2}{\pi s}}\Big\{ \quad \cos(s-\frac{\pi}{4})\big[\frac{1}{2} + \frac{R_4(\beta,\kappa)}{(8s)^2}\big] + \sin(s-\frac{\pi}{4})\big[\frac{R_2(\beta,\kappa)}{(8s)}\big]\Big\} + O(s^{-\frac{7}{2}}) \ , \quad \text{(E.28)}$$

where

$$R_2(\beta,\kappa) = \frac{9+\epsilon^2(\beta,\kappa)}{2[1+\epsilon^2(\beta,\kappa)]} \ , \quad \text{(E.29)}$$

$$R_4(\beta,\kappa) = -\frac{9}{4} + \frac{12}{1+\epsilon^2(\beta,\kappa)} - \frac{96}{(1+\epsilon^2(\beta,\kappa))^2} \ . \quad \text{(E.30)}$$

With Eq. (E.28) we now have an asymptotic expansion for $I(\epsilon, s)$, which leads to the following expressions for $\Lambda_0(\beta w, s)$ and $\Lambda_1(\beta w, s)$:

$$\begin{aligned}\Lambda_0(\beta w, s) \ \approx \ & \frac{J_0(s)}{2} + \sigma_1(\beta,\kappa)\frac{e^{-\epsilon(\beta,\kappa)s}}{\sqrt{1+\epsilon^2(\beta,\kappa)}} \\ + \ & \sigma_1(\beta,\kappa)\sqrt{\frac{2}{\pi s}}\frac{\epsilon(\beta,\kappa)}{1+\epsilon^2(\beta,\kappa)}\Big\{\cos(s-\frac{\pi}{4})\big[1+\frac{2R_4(\beta,\kappa)}{(8s)^2}\big] \\ + \ & \sin(s-\frac{\pi}{4})\big[\frac{2R_2(1,\kappa)}{8s}\big]\Big\} + \frac{\sigma_1(\beta,\kappa)}{\sqrt{1+\epsilon^2(\beta,\kappa)}}O(s^{-\frac{7}{2}}),\end{aligned} \quad \text{(E.31)}$$

$$\begin{aligned}\Lambda_1(\beta w, s) \ \approx \ & \frac{\epsilon(\beta,\kappa)\sigma_2(\beta,\kappa)}{\sqrt{1+\epsilon^2(\beta,\kappa)}}\Big\{e^{-\epsilon(\beta,\kappa)s} - \frac{1}{\sqrt{1+\epsilon^2(\beta,\kappa)}}\sqrt{\frac{2}{\pi s}} \times \\ \times \ & \Big[\cos(s-\frac{\pi}{4})\big(\frac{2[R_2(\beta,\kappa)-2]}{8s} - 40\frac{R_4(\beta,\kappa)}{(8s)^3}\big) \\ - \ & \sin(s-\frac{\pi}{4})\big(1+\frac{2[R_4(\beta,\kappa)+12R_2(\beta,\kappa)]}{(8s)^2}\big)\Big]\Big\} \\ + \ & \frac{\epsilon(\beta,\kappa)\sigma_2(\beta,\kappa)}{1+\epsilon^2(\beta,\kappa)}O(s^{-\frac{9}{2}}) \ ,\end{aligned} \quad \text{(E.32)}$$

Appendix F

Thermal Averages and Correlation Functions

In Chapter 6 we require the thermal average of several functions of the normal mode amplitudes b_k. In general the b_k's are complex and we use for convenience the following definition for the averages

$$\langle F(b_q, b^*_{q'})\rangle = \frac{\prod\limits_k \int\limits_{-\infty}^{\infty} db_k \int\limits_{-\infty}^{\infty} db^*_k \ F(b_q, b^*_{q'}) e^{-\beta\omega_k |b_k|^2}}{\prod\limits_k \int\limits_{-\infty}^{\infty} db_k \int\limits_{-\infty}^{\infty} db^*_k \ e^{-\beta\omega_k |b_k|^2}} \tag{F.1}$$

From this definition it is clear that $\langle b_k\rangle = \langle b^*_k\rangle = 0$. However, to see that quantities such as $\langle b^2_k\rangle = \langle {b_k}^{*2}\rangle = 0$ it is useful to write the average in terms of the real and imaginary parts, for example

$$\langle b^2_k\rangle = \langle {b^R_k}^2 + 2b^R_k b^I_k - {b^I_k}^2\rangle \ . \tag{F.2}$$

The average in terms of the real and imaginary parts becomes

$$\langle F(b_q, b^*_{q'})\rangle = \frac{\prod\limits_k \int\limits_{-\infty}^{\infty} db^R_k \int\limits_{-\infty}^{\infty} db^I_k \ F(b_q, b_{q'}) e^{-\beta\omega_k ({b^R_k}^2 + {b^I_k}^2)}}{\prod\limits_k \int\limits_{-\infty}^{\infty} db^R_k \int\limits_{-\infty}^{\infty} db^I_k \ e^{-\beta\omega_k ({b^R_k}^2 + {b^I_k}^2)}} \ , \tag{F.3}$$

from which we can see that the cross term in Eq. (F.2) is zero and the quadratic terms are equal.

In general the complex notation is easier to handle which may be illustrated by the ease with which $\langle b_q b^*_q\rangle$ is computed:

$$\langle b_q b^*_q\rangle = \frac{\prod\limits_k \int\limits_{-\infty}^{\infty} db_k \int\limits_{-\infty}^{\infty} db^*_k |b_q|^2 e^{-\beta\omega_k |b_k|^2}}{\prod\limits_k \int\limits_{-\infty}^{\infty} db_k \int\limits_{-\infty}^{\infty} db^*_k e^{-\beta\omega_k |b_k|^2}} \ , \tag{F.4}$$

$$= \frac{\int\limits_0^\infty |b_q|^2 e^{-\beta\omega_q |b_q|^2} d|b_q|^2}{\int\limits_0^\infty e^{-\beta\omega_q |b_q|^2} d|b_q|^2} , \tag{F.5}$$

$$= \frac{T}{\omega_q} , \tag{F.6}$$

where we have made a transformation to polar coordinates and taken k_B to be 1. With these averages computed we can compute some of the more complicated averages and correlations. The first of these is the average of ψ^2 which is

$$\begin{aligned} \langle \psi^2(x,t) \rangle &= \Big\langle \sum_{k_1,k_2} \Big[b_{k_1} f_{k_1}(x) e^{-i\omega_{k_1} t} + b^*_{k_1} f^*_{k_1}(x) e^{i\omega_{k_1} t} \Big] \times \\ &\times \Big[b_{k_2} f_{k_2}(x) e^{-i\omega_{k_2} t} + b^*_{k_2} f^*_{k_2}(x) e^{i\omega_{k_2} t} \Big] \Big\rangle , &\text{(F.7)} \\ &= \sum_k \frac{\langle b_k b^*_k \rangle |f_k(x)|^2}{\omega_k} , &\text{(F.8)} \\ &= T \sum_k \frac{|f_k(x)|^2}{\omega_k^2} . &\text{(F.9)} \end{aligned}$$

The sum in Eq. (F.9) is exactly the static Green function. Using the sine-Gordon static Green function [115] we can write

$$\langle \psi^2(x,t) \rangle = \frac{T}{2} \Big(1 - \frac{1}{2} \mathrm{sech}^2 x \Big) . \tag{F.10}$$

Next we use the fact that the functions $f_k(x)$ have the following symmetry

$$f_k(-x) = \pm f_{-k}(x) , \tag{F.11}$$

which tells us that

$$\langle \psi^2(-x,t) \rangle = \langle \psi^2(x,t) \rangle . \tag{F.12}$$

Next using the fact that $U'''[\phi_c(-x)] = -U'''[\phi_c(x)]$ and $\phi'_c(-x) = \phi'_c(x)$ we have [recall Eq. (6.1.3) for F_ψ]

$$\langle F_\psi \rangle = \frac{1}{2M_0} \int\limits_{-\infty}^{\infty} U'''[\phi_c(x)] \phi'_c(x) \langle \psi^2(x,t) \rangle = 0 . \tag{F.13}$$

Also since η_ψ [see Eq. (6.1.2)] is linear in ψ we have

$$\langle \eta_\psi \rangle = 0 . \tag{F.14}$$

Now we go on to compute the correlation functions $\langle \eta_\psi(t)\ \eta_\psi(t')\rangle$ and $\langle F_\psi(t)\ F_\psi(t')\rangle$. First we consider the η correlation function which we write as

$$\begin{aligned}\langle \eta_\psi(t)\ \eta_\psi(t')\rangle &= \frac{4}{M_0^2}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \phi_c''(x)\phi_c''(x') \times \\ &\quad \times \sum_k \left[\frac{\omega_k}{2}\langle b_k b_k^*\rangle f_k(x) f_k^*(x') e^{-i\omega_k(t-t')} + H.C.\right] \quad \text{(F.15)} \\ &= \frac{2T}{M_0^2}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \phi_c''(x)\phi_c''(x') \times \\ &\quad \times \sum_k \left[f_k(x) f_k^*(x') e^{-i\omega_k(t-t')} + H.C.\right] \quad \text{(F.16)} \\ &= \frac{4T}{M_0^2}\sum_k \Big|\int dx \phi_c''(x) f_k(x)\Big|^2 \cos[\omega_k(t-t')]\ . \quad \text{(F.17)}\end{aligned}$$

For $t - t' > 1/\omega_{k_0}$ this correlation function decays rapidly where ω_{k_0} is the lowest frequency and $H.C.$ means Hermitian conjugate.

The last correlation function computed is $\langle F_\psi(t)\ F_\psi(t')\rangle$ where $F_\psi(t)$ in terms of normal mode amplitudes is given by

$$\begin{aligned}F_\psi &= \frac{1}{2M_0}\int dx U'''[\phi_c(x)]\phi_c'(x) \sum_{k_1,k_2}\frac{1}{\sqrt{4\omega_{k_1}\omega_{k_2}}}\Big\{ b_{k_1} b_{k_2} f_{k_1}(x) f_{k_2}(x) e^{-i(\omega_{k_1}+\omega_{k_2})t} \\ &+ \qquad b_{k_1} b_{k_2}^* f_{k_1}(x) f_{k_2}^*(x) e^{-i(\omega_{k_1}-\omega_{k_2})t} + \ H.C.\Big\}\ . \quad \text{(F.18)}\end{aligned}$$

In doing the average only those terms which have two b_k's and b_k^*'s are nonzero; therefore we write

$$\langle F_\psi(t)\ F_\psi(t')\rangle = \frac{1}{2M_0}\int dx U'''[\phi_c(x)]\phi_c'(x) \int dx' U'''[\phi_c(x')]\phi_c'(x') \Big[A + B + H.C.\Big]\ , \quad \text{(F.19)}$$

with A and B given by

$$A = \sum_{k_1,k_2,k_3,k_4} \frac{\langle b_{k_1} b_{k_2} b_{k_3}^* b_{k_4}^*\rangle}{\sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}} f_{k_1}(x) f_{k_2}(x) f_{k_3}^*(x') f_{k_4}^*(x') e^{-i(\omega_{k_1}+\omega_{k_2})t + i(\omega_{k_3}+\omega_{k_4})t'}\ , \quad \text{(F.20)}$$

$$B = \sum_{k_1,k_2,k_3,k_4} \frac{\langle b_{k_1} b_{k_2}^* b_{k_3} b_{k_4}^*\rangle}{\sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}} f_{k_1}(x) f_{k_2}^*(x) f_{k_3}(x') f_{k_4}^*(x') e^{-i(\omega_{k_1}-\omega_{k_2})t - i(\omega_{k_3}-\omega_{k_4})t'}\ . \quad \text{(F.21)}$$

First we consider the A term. The averages of the four b factors is zero unless $k_1 = k_3, k_2 = k_4$ or $k_1 = k_4, k_2 = k_3$, both of which are the same due to relabeling and therefore we restrict ourselves to the former. First we consider $k_1 = k_3, k_2 = k_4$ but $k_1 \neq k_4$ in which the average over the b_{k_i} factors yields

$$\langle |b_{k_1}|^2 |b_{k_3}|^2 \rangle = \frac{T}{\omega_{k_1}} \frac{T}{\omega_{k_2}} \ . \tag{F.22}$$

Therefore this contribution to A can be written as

$$2 \sum_{k_1,k_2} \frac{T^2}{\omega_{k_1}^2 \omega_{k_2}^2} f_{k_1}(x) f_{k_1}^*(x') f_{k_2}(x) f_{k_2}^*(x') e^{-i(\omega_{k_1}+\omega_{k_2})(t-t')} \ , \tag{F.23}$$

where the factor of 2 is due to the $k_1 = k_4, k_2 = k_3$ term. In the case that $k_1 = k_2 = k_3 = k_4$ we must evaluate

$$\begin{aligned} \langle |b_k|^4 \rangle &= \frac{\int_0^\infty |b_k|^4 e^{-\beta\omega_k |b_k|^2} d|b_k|^2}{\int_0^\infty e^{-\beta\omega_k |b_k|^2} d|b_k|^2} \ , & \text{(F.24)} \\ &= \frac{2T^2}{\omega_k^2} \ , & \text{(F.25)} \end{aligned}$$

which leads to the following contribution to A

$$2 \sum_{k_1,k_2} \delta_{k_1,k_2} \frac{T^2}{\omega_{k_1}^2 \omega_{k_2}^2} f_{k_1}(x) f_{k_1}^*(x') f_{k_2}(x) f_{k_2}^*(x') e^{-i(\omega_{k_1}+\omega_{k_2})(t-t')} \ , \tag{F.26}$$

which allows us to write for A

$$A = 2 \sum_{k_1,k_2} \frac{T^2}{\omega_{k_1}^2 \omega_{k_2}^2} f_{k_1}(x) f_{k_1}^*(x') f_{k_2}(x) f_{k_2}^*(x') e^{-i(\omega_{k_1}+\omega_{k_2})(t-t')} \ , \tag{F.27}$$

Similarly for the B term we consider the terms with $k_1 = k_2, k_3 = k_4$ but $k_1 \neq k_3$ (not the same as $k_1 = k_4, k_2 = k_3$) which yields the contribution

$$\begin{aligned} \sum_{k_1 \neq k_3} \frac{T^2}{\omega_{k_1}\omega_{k_3}} |f_{k_1}(x)|^2 |f_{k_3}(x')|^2 &= \sum_{k_1,k_3} \frac{T^2}{\omega_{k_1}\omega_{k_3}} |f_{k_1}(x)|^2 |f_{k_3}(x')|^2 - \\ & \sum_k \frac{T^2}{\omega_k^2} |f_k(x)|^2 |f_k(x')|^2 \ . & \text{(F.28)} \end{aligned}$$

Before we compute the other contributions to B we note that when the required integrals over space are done to complete the calculation of $\langle F_\psi(t)\ F_\psi(t') \rangle$, the first term of Eq. (F.27) may be written as

$$\left[\int_{-\infty}^{\infty} dx U'''[\phi_c(x)] \phi_c'(x) \sum_k \frac{T}{\omega_k^2} |f_k(x)|^2 \right]^2 \ , \tag{F.29}$$

which is zero since the integrand is odd upon the interchange $x \to -x$, $k \to -k$. The term for which $k_1 = k_4, k_2 = k_3$ but $k_1 \neq k_2$ can be written as

$$\sum_{k_1 \neq k_2} \frac{T^2}{\omega_{k_1}\omega_{k_2}} f_{k_1}(x) f^*_{k_1}(x') f^*_{k_2}(x) f_{k_2}(x') e^{-i(\omega_{k_1}-\omega_{k_2})(t-t')} \ . \qquad \text{(F.30)}$$

Finally, evaluation of the $k_1 = k_2 = k_3 = k_4$ term yields exactly $-1/2$ of the second term in Eq. (F.27), which when combined with Eq. (F.29) yields

$$B = \sum_{k_1,k_2} \frac{T^2}{\omega^2_{k_1}\omega^2_{k_2}} f_{k_1}(x) f^*_{k_1}(x') f^*_{k_2}(x) f_{k_2}(x') e^{-i(\omega_{k_1}-\omega_{k_2})(t-t')} \ . \qquad \text{(F.31)}$$

Next we use the fact that $f_{-k}(x) = \pm f^*_k(x)$ which allows us to write

$$B = \sum_{k_1,k_2} \frac{T^2}{\omega^2_{k_1}\omega^2_{k_2}} f_{k_1}(x) f^*_{k_1}(x') f_{k_2}(x) f^*_{k_2}(x') e^{-i(\omega_{k_1}-\omega_{k_2})(t-t')} \ , \qquad \text{(F.32)}$$

which is the same as $A/2$ except for the exponential in time. Combining these factors we have

$$\begin{aligned} \langle F_\psi(t)\ F_\psi(t')\rangle &= \frac{1}{4M_0^2} \int dx U'''[\phi_c(x)]\phi'_c(x) \int dx' U'''[\phi_c(x')]\phi'_c(x') \times \\ &\times \sum_{k_1,k_2} \frac{T^2}{\omega^2_{k_1}\omega^2_{k_2}} f_{k_1}(x) f^*_{k_1}(x') f_{k_2}(x) f^*_{k_2}(x') \times \\ &\times \left\{ e^{-i(\omega_{k_1}+\omega_{k_2})(t-t')} + e^{-i(\omega_{k_1}-\omega_{k_2})(t-t')} \right\} + H.C. \qquad \text{(F.33)} \end{aligned}$$

We can obtain further simplification by recalling that the functions $f_k(x)$ obey

$$-f''_k(x) + U''[\phi_c(x)] f_k(x) = \omega_k^2 f_k(x) \qquad \text{(F.34)}$$

which allows us to rewrite the integrals in Eq. (F.33) as

$$\begin{aligned} &\int dx U'''[\phi_c(x)]\phi'_c(x) f_{k_1}(x) f_{k_2}(x) \\ &= \int dx f_{k_1}(x) f_{k_2}(x) \frac{dU''[\phi_c(x)]}{dx} \qquad \text{(F.35)} \\ &= -\int dx U''[\phi_c(x)] \Big[f'_{k_1}(x) f_{k_2}(x) + f_{k_1}(x) f'_{k_2}(x) \Big] \qquad \text{(F.36)} \\ &= \int \Big\{ f'_{k_1}(x) \Big[f''_{k_2}(x) + \omega^2_{k_2} f_{k_2} \Big] + f'_{k_2}(x) \Big[f''_{k_1}(x) + \omega^2_{k_1} f_{k_1} \Big] \Big\} dx \qquad \text{(F.37)} \\ &= \int \Big\{ \frac{d}{dx} \Big[f'_{k_1}(x) f'_{k_2}(x) \Big] + (\omega^2_{k_1} - \omega^2_{k_2}) f_{k_1}(x) f'_{k_2}(x) \\ &\qquad + \frac{d}{dx} \Big[f_{k_1}(x) f'_{k_2}(x) \Big] \omega^2_{k_2} \Big\} dx \qquad \text{(F.38)} \\ &= (\omega^2_{k_1} - \omega^2_{k_2}) \int dx f_{k_1}(x) f'_{k_2}(x) \ , \qquad \text{(F.39)} \end{aligned}$$

where the surface terms vanish by periodic boundary conditions. Finally we have

$$\begin{aligned}\langle F_\psi(t)\ F_\psi(t')\rangle &= \frac{T^2}{2M_0^2}\sum_{k_1,k_2}\frac{(\omega_{k_1}^2-\omega_{k_2}^2)^2}{\omega_{k_1}^2\omega_{k_2}^2}\Big|\int dx f_{k_1}(x) f'_{k_2}(x)\Big|^2 \times \\ &\times \Big[\cos[(\omega_{k_1}+\omega_{k_2})(t-t')] + \cos[(\omega_{k_1}-\omega_{k_2})(t-t')]\Big]\ . \end{aligned} \quad \text{(F.40)}$$

Appendix G

Functional Derivatives in Terms of Kink Variables

In order to derive the Fokker-Planck equation in Appendix H for the kink variables X and p we need to have expressions for the derivatives with respect to $\Phi(x,t)$ and $\Pi_0(x,t)$ in terms of the new variables $\{X, p, \psi, \pi\}$. The fact that this transformation is nontrivial may be seen recalling that the ψ field is constrained to be in the subspace which is perpendicular to $\phi_c(x)$. Therefore, when we take a functional derivative with respect to ψ it must be understood to include only variations in that subspace. To see how to take such "constrained" derivatives, it is useful to examine what is meant when a "regular" functional derivative is taken. Consider for example the derivative of a field $F[\Phi(x,t)]$ with respect to $\Phi(x',t')$

$$\frac{\delta F[\Phi(x,t)]}{\delta\Phi(x',t')} \equiv \lim_{\epsilon\to 0} \frac{F[\Phi(x,t)+\epsilon\delta(x-x')] - F[\Phi(x,t)]}{\epsilon} \ . \tag{G.1}$$

From this definition, it is clear what is meant by a derivative which is constrained to the subspace perpendicular to $\phi_c(x)$, namely

$$\frac{\delta F[\psi(x,t)]}{\delta\psi(x',t')} = \lim_{\epsilon\to 0} \frac{F[\Phi(x,t)+\epsilon\delta(x-x') - \epsilon\frac{\phi_c'(x)\phi_c'(x')}{M_0}] - F[\Phi(x,t)]}{\epsilon} \ . \tag{G.2}$$

In subtracting the "translation mode" term we allow only variations which are in the ψ subspace. In particular we have the following derivatives,

$$\frac{\delta\psi(x,t)}{\delta\psi(x',t')} = \delta(x-x')\delta(t-t') - \frac{\phi_c'(x)\phi_c'(x')}{M_0}\delta(t-t') \ , \tag{G.3}$$

$$\frac{\delta\pi(x,t)}{\delta\pi(x',t')} = \delta(x-x')\delta(t-t') - \frac{\phi_c'(x)\phi_c'(x')}{M_0}\delta(t-t') \ , \tag{G.4}$$

which follow from Eq. (G.2). In writing these "constrained" derivatives, one should be able to avoid the use of Dirac brackets by using the standard Poisson brackets with the derivatives understood to mean the constrained derivatives. As a check we compute the *Poisson* bracket of $\psi(x,t)$ with $\pi(y,t)$ using the constrained derivatives:

$$\begin{aligned}
&\{\psi(x,t),\pi(y,t)\} \\
&= \int_{-\infty}^{\infty} dz \left[\frac{\delta\psi(x,t)}{\delta\psi(z,t)}\frac{\delta\pi(y,t)}{\delta\pi(z,t)} - \frac{\delta\psi(x,t)}{\delta\pi(z,t)}\frac{\delta\pi(y,t)}{\delta\psi(z,t)}\right] , \qquad \text{(G.5)} \\
&= \int_{-\infty}^{\infty} dz \left(\delta(x-z) - \frac{\phi_c'(x)\phi_c'(z)}{M_0}\right)\left(\delta(y-z) - \frac{\phi_c'(y)\phi_c'(z)}{M_0}\right) , \qquad \text{(G.6)} \\
&= \delta(x-y) - 2\frac{\phi_c'(x)\phi_c'(y)}{M_0} + \frac{\phi_c'(x)\phi_c'(y)}{M_0^2}\int_{-\infty}^{\infty} dz\ \phi_c'(z)\phi_c'(z) \ , \qquad \text{(G.7)} \\
&= \delta(x-y) - \frac{\phi_c'(x)\phi_c'(y)}{M_0} , \qquad \text{(G.8)}
\end{aligned}$$

which is exactly the *Dirac* bracket of $\psi(x,t)$ with $\pi(y,t)$.

With the identities (G.3) and (G.4) in hand we proceed to derive the derivatives with respect to $\Phi(x,t)$ and $\Pi_0(x,t)$. This is accomplished by writing the most general transformation between the variables and requiring the identities

$$\frac{\delta\Phi(x,t)}{\delta\Phi(x',t')} = \delta(x-x')\delta(t-t') \qquad \frac{\delta\Phi(x,t)}{\delta\Pi_0(x',t')} = 0 \qquad \text{(G.9)}$$

$$\frac{\delta\Pi_0(x,t)}{\delta\Phi(x',t')} = 0 \qquad \frac{\delta\Pi_0(x,t)}{\delta\Pi_0(x',t')} = \delta(x-x')\delta(t-t') \ . \qquad \text{(G.10)}$$

First we consider the Φ derivative which may be assumed to have the following form which is linear in derivatives with respect to kink variables:

$$\begin{aligned}
\frac{\delta}{\delta\Phi(x',t')} &= \int dt'' A(x',t',t'')\frac{\delta}{\delta X(t'')} + \int dx''dt'' B(x',t',x'',t'')\frac{\delta}{\delta\psi(\zeta'',t'')} \\
&+ \int dt'' C(x',t',t'')\frac{\delta}{\delta p(t'')} + \int dx''dt'' D(x',t',x'',t'')\frac{\delta}{\delta\pi(\zeta'',t'')} \qquad \text{(G.11)}
\end{aligned}$$

with ζ defined by

$$\zeta \equiv x - X \ . \qquad \text{(G.12)}$$

Operating on $\Phi(x,t)$ with Eq. (G.9) yields

$$\begin{aligned}
\delta(x-x')\delta(t-t') = &-[\phi_c'(\zeta)+\psi'(\zeta,t)]A(x',t',t) + B(x',t',x,t) \\
&-\frac{\phi_c'(\zeta)}{M_0}\int dx''\ B(x',t',x'',t)\phi_c'(\zeta'') \ .
\end{aligned} \qquad \text{(G.13)}$$

Multiplying Eq. (G.13) by $\phi_c'(\zeta)$ and integrating over ζ gives us

$$A(x',t',t) = -\frac{\phi_c'(\zeta')}{M_0+\xi(t')}\delta(t-t') \ . \tag{G.14}$$

Multiplying Eq. (G.13) by $\psi(\zeta,t)$ and integrating over ζ gives us

$$\psi(\zeta',t)\delta(t-t') = \int dx'' B(x',t',x'',t)\Big[\psi(\zeta'',t) - \frac{\xi(t)}{M_0}\phi_c'(\zeta'')\Big] \tag{G.15}$$

The solution to this integral equation is

$$\begin{aligned} B(x',t',x'',t'') = \delta(t'-t'')\Bigg\{\delta(x'-x'') \quad &- \quad \frac{\phi_c'(\zeta')\phi_c'(\zeta'')}{M_0} - \frac{\phi_c'(\zeta')\psi'(\zeta'')}{M_0+\xi(t)} \\ &+ \quad \frac{\phi_c'(\zeta')\phi_c'(\zeta'')\xi(t)}{M_0(M_0+\xi(t))}\Bigg\} \ . \end{aligned} \tag{G.16}$$

When this expression for B is substituted into Eq. (G.13) we see that the terms proportional to $\phi_c'(\zeta'')$ are not necessary since the derivative

$$\frac{\delta\psi(\zeta,t)}{\delta\psi(\zeta',t')} \ , \tag{G.17}$$

is manifestly orthogonal to $\phi_c'(\zeta)$. Therefore the expression for B is effectively

$$B(x',t',x'',t'') = \delta(t'-t'')\left\{\delta(x'-x'') - \frac{\phi_c'(\zeta')\psi'(\zeta'')}{M_0+\xi(t)}\right\} \ . \tag{G.18}$$

The functions $C(x',t',t'')$ and $D(x',t',x'',t'')$ are obtained by operating on $\Pi_0(x',t')$ with Eq. (G.11) which yields after quite a bit of algebra

$$\begin{aligned} 0 \quad &= \quad \frac{1}{M_0+\xi(t)}\Big[\phi_c'(\zeta')\Pi_0'(x,t) + \phi_c'(\zeta)\Pi_0'(x',t)\Big] - \frac{\phi_c'(\zeta')\phi_c'(\zeta)}{(M_0+\xi(t))^2}\int dx\ \Pi_0'\Phi' \\ &- \quad \frac{\phi_c'(\zeta)C(x',t',t)}{M_0+\xi(t)} + D(x',t',x,t) - \frac{\phi_c'(\zeta)}{M_0}\int dx'' D(x',t',x'',t)\phi_c'(\zeta'') \\ &- \quad \frac{\phi_c'(\zeta)}{M_0+\xi(t)}\left[\psi'(\zeta',t) - \frac{\xi(t)}{M_0}\phi_c'(\zeta'')\right] \ . \end{aligned} \tag{G.19}$$

Multiplying Eq. (G.19) by $\phi_c'(\zeta)$ and $\psi(\zeta,t)$ and integrating over ζ yields

$$\begin{aligned} 0 \quad &= \quad \frac{M_0}{M_0+\xi(t)}\Pi_0'(x',t) + \frac{\phi_c'(\zeta')}{M_0+\xi(t)}\int dx'\ \Pi_0'(x',t)\phi_c'(\zeta') \\ &- \quad \frac{M_0\phi_c'(\zeta')}{(M_0+\xi(t))^2}\int dx'\ \Pi_0'(x',t)\Phi'(x',t) - \frac{M_0}{M_0+\xi(t)}C(x',t',t) \\ &- \quad \frac{M_0}{M_0+\xi(t)}\int dx'' D(x',t',x'',t)\left[\psi'(\zeta'',t) - \frac{\xi(t)}{M_0}\phi_c'(\zeta'')\right] \ , \end{aligned} \tag{G.20}$$

and

$$
\begin{aligned}
0 &= -\frac{\xi(t)}{M_0+\xi(t)}C(x',t',t) + \frac{M_0}{M_0+\xi(t)}\int dx'' D(x',t',x'',t)\psi'(\zeta'',t) \\
&- \frac{\xi(t)}{M_0+\xi(t)}\int dx'' D(x',t',x'',t)\phi_c'(\zeta'',t) + \frac{\xi(t)}{M_0+\xi(t)}\Pi_0'(x,t) \\
&+ \frac{M_0\phi_c'(\zeta)}{(M_0+\xi(t))^2}\int dx'\ \Pi_0'(x',t)\Phi'(x,t) - \frac{\phi_c'(\zeta')}{M_0+\xi(t)}\int dx'\Pi_0'(x',t)\phi_c'(\zeta')\ ,
\end{aligned}
\tag{G.21}
$$

where the second of these equations was obtained after a bit of algebra. In Eq. (G.20) we solve for $C(x',t',t)$ and substitute this into Eq. (G.21) which, after some manipulations, gives us

$$
\begin{aligned}
0 &= \int dx'' D(x',t',x'',t)\left[\psi'(\zeta',t) - \frac{\xi(t)}{M_0}\phi_c'(\zeta'')\right] \\
&+ \frac{\phi_c'(\zeta)}{M_0+\xi(t)}\int dx''\Pi_0'(x'',t)\left[\psi'(\zeta',t) - \frac{\xi(t)}{M_0}\phi_c'(\zeta'')\right]\ ,
\end{aligned}
\tag{G.22}
$$

from which we deduce

$$
D(x',t',x'',t'') = -\frac{\phi_c'(\zeta')}{M_0+\xi(t)}\Pi_0'(x'',t)\ . \tag{G.23}
$$

Substitution of this expression for D into Eq. (G.21) yields

$$
C(x',t',t) = \Pi_0'(x',t)\delta(t-t') \tag{G.24}
$$

Collecting these calculations we have

$$
\begin{aligned}
\frac{\delta}{\delta\Phi(x',t')} &= -\frac{\phi_c'(\zeta')}{M_0+\xi(t')}\frac{\delta}{\delta X(t'')} + \int dx''\left\{\delta(x'-x'') - \frac{\phi_c'(\zeta')\psi'(\zeta'')}{M_0+\xi(t)}\right\}\frac{\delta}{\delta\psi(\zeta'')} \\
&+ \Pi_0'(x',t)\frac{\delta}{\delta p(t')} - \frac{\phi_c'(\zeta')}{M_0+\xi(t')}\int\ dx''\ \Pi_0'(x'',t)\frac{\delta}{\delta\pi(\zeta'')}\ .
\end{aligned}
\tag{G.25}
$$

We derive the analogous expression for the Π_0 derivative by using the same methods. For the sake of brevity we merely present the result,

$$
\frac{\delta}{\delta\Pi_0(x',t')} = -\Phi'(x',t')\frac{\delta}{\delta p(t')} + \frac{\delta}{\delta\pi(\zeta')}\ , \tag{G.26}
$$

where in both of the final expressions the full fields Φ and Π_0 are used to achieve a more compact notation.

Appendix H

Fokker-Planck Equation for $P(X, p; t)$

In this appendix we derive a Fokker Planck equation for the phase space distribution function $P(X, p; t)$ (see Chapter 6) by starting from the full field equation

$$\frac{\partial P(\Phi, \Pi_0; t)}{\partial t} = \int_{-\infty}^{\infty} dx \Big\{ -\Pi_0 \frac{\delta}{\delta \Phi} P(\Phi, \Pi_0; t) - \frac{\delta}{\delta \Pi_0} \Big[\Big(\Phi_{xx} - U'[\Phi] - \epsilon \Pi_0 \Big) P(\Phi, \Pi_0; t) \Big] + \epsilon k_B T \frac{\delta^2}{\delta \Pi_0^2} P(\Phi, \Pi_0; t) \Big\} , \quad \text{(H.1)}$$

substituting the ansatz

$$P[\Phi, \Pi_0; t] = e^{-\beta H_{ph}} P(X, p; t) , \quad \text{(H.2)}$$

with

$$H_{ph} = \int \Big[\frac{1}{2}\pi^2 + \frac{1}{2}\psi'^2 + \frac{1}{2}\psi^2 U''(\phi_c) \Big] . \quad \text{(H.3)}$$

and then using the results of Appendix G, we take the functional derivatives in Eq. (H.1) in terms of the kink variables. We shall consider each term in Eq. (H.1) separately to avoid extremely long expresssions. Using Eq. (G.25) the first term becomes

$$-\int dx \Pi_0 \frac{\delta P[\Phi, \Pi_0; t]}{\delta \Phi} = - \int dx \; \Pi_0 \Big\{ -\frac{\phi_c'(\zeta)}{M_0 + \xi} \frac{\delta P(X, p; t)}{\delta X} - \beta \int dx'' \Big[\delta(x - x'') - \frac{\phi_c'(\zeta)\psi'(\zeta'')}{M_0 + \xi} \Big] \times P(X, p; t) \frac{\delta H_{ph}}{\delta \psi(\zeta'', t)} + \beta \frac{\phi_c'(\zeta)}{M_0 + \xi} \int dx'' \; \Pi_0' \frac{\delta H_{ph}}{\delta \pi(\zeta'', t)} \Big\} . \quad \text{(H.4)}$$

First consider the derivative with respect to ψ

$$\begin{aligned}
&\frac{\delta H_{ph}}{\delta\psi(\zeta'',t)} \\
&= \int dx' \frac{\delta}{\delta\psi(\zeta'',t)}\Big[\frac{1}{2}\psi'^2(\zeta',t)+\frac{1}{2}\psi^2(\zeta',t)U''(\phi_c)\Big] && \text{(H.5)}\\
&= \int dx'\Big[-\psi''(\zeta',t)+\psi(\zeta',t)U''(\phi_c)\Big]\Big[\delta(x'-x'')-\frac{\phi_c'(\zeta')\phi_c'(\zeta'')}{M_0}\Big] && \text{(H.6)}\\
&= -\psi''(\zeta'',t)+\psi(\zeta'',t)U''[\phi_c(\zeta'')] \ , && \text{(H.7)}
\end{aligned}$$

where we have repeatedly made use of the constraints (Eq. (3.3.10-11)) and the fact that $\phi_c'' = U'(\phi_c)$. Substituting this expression into the first integration over x'' in Eq. (H.4), we have

$$\begin{aligned}
\int dx''\Big[\delta(x-x'')-\frac{\phi_c'(\zeta)\psi'(\zeta'')}{M_0+\xi}\Big]\frac{\delta H_{ph}}{\delta\psi(\zeta'',t)} &= \\
- \quad \psi''(\zeta,t)+\psi(\zeta,t)U''[\phi_c(\zeta)] \\
- \quad \phi_c'(\zeta)\frac{\xi}{M_0}\Big[-\int \phi_c'\psi''+\phi_c'\psi U''(\phi_c)\Big] && \text{(H.8)}\\
= \quad -\psi''(\zeta,t)+\psi(\zeta,t)U''[\phi_c(\zeta)] \ . && \text{(H.9)}
\end{aligned}$$

Next we examine the π derivative term:

$$-\int dx\Pi_0(x,t)\frac{\phi_c(\zeta')}{M_0+\xi}\int dx''\Pi_0'(x'',t)\frac{\delta H_{ph}}{\delta\pi(\zeta'',t)} \ . \qquad \text{(H.10)}$$

The derivative of H_{ph} with respect to π will bring down another factor of π which results in the product of three momentum fields. Keeping terms of this order is not consistent with the phonon ansatz made and therefore we do not include this term. Collecting these results we have for the first term

$$\begin{aligned}
&\int_{-\infty}^{\infty} -\Pi_0\frac{\delta}{\delta\Phi}P(\Phi,\Pi_0;t) \\
&= \frac{M_0(p+\int\pi\psi')}{(M_0+\xi)^2}e^{-\beta H_{ph}}\frac{\delta P(X,p;t)}{\delta X}+\beta e^{-\beta H_{ph}}P(X,p;t)\int\Pi_0(\psi''-\psi U'(\phi_c)) \ . && \text{(H.11)}
\end{aligned}$$

Using the fact that

$$\frac{\delta H_{ph}}{\delta\Pi_0} = \pi \ , \qquad \text{(H.12)}$$

we easily find that

$$
\begin{aligned}
-\int dx \frac{-\delta}{\delta \Pi_0}\Big[\Phi_{xx} - U'(\Phi) - \epsilon \Pi_0\Big] e^{-\beta H_{ph}} P(X,p;t) = \\
- \quad & \beta P(X,p;t) e^{-\beta H_{ph}} \int dx\ \pi \Big[-\psi'' + \psi U'(\phi_c)\Big] + \epsilon \int dx\ \frac{-\delta}{\delta \Pi_0}\Big[\pi e^{-\beta H_{ph}} P(X,p;t)\Big] \\
+ \quad & \epsilon\ e^{-\beta H_{ph}} \frac{\delta}{\delta p} p P(X,p;t)\ . \qquad \text{(H.13)}
\end{aligned}
$$

Finally we have for the last term

$$
\begin{aligned}
& \frac{\epsilon}{\beta} \int dx \frac{\delta^2}{\delta \Pi_0^2}\Big[e^{-\beta H_{ph}} P(X,p;t)\Big] \\
= \quad & -\epsilon \int dx \frac{\delta}{\delta \Pi_0}\Big[\pi e^{-\beta H_{ph}} P(X,p;t)\Big] - \frac{\epsilon}{\beta} \int dx \frac{\delta}{\delta \Pi_0}\Big[\Phi' e^{-\beta H_{ph}} \frac{\delta P(X,p;t)}{\delta p}\Big] \qquad \text{(H.14)} \\
= \quad & -\epsilon \int dx \frac{\delta}{\delta \Pi_0}\Big[\pi e^{-\beta H_{ph}} P(X,p;t)\Big] \\
+ \quad & \frac{\epsilon}{\beta}\Big[\int \Phi'\Phi'\Big] e^{-\beta H_{ph}} \frac{\delta^2 P(X,p;t)}{\delta p^2} + \epsilon \Big(\int \psi' \pi\Big) e^{-\beta H_{ph}} \frac{\delta P(X,p;t)}{\delta p}\ . \qquad \text{(H.15)}
\end{aligned}
$$

Combining all three contributions we have

$$
\begin{aligned}
& e^{-\beta H_{ph}} \frac{\partial P(X,p;t)}{\partial t} \\
= \quad & e^{-\beta H_{ph}} \Bigg\{ \frac{p + \int \pi \psi'}{M_0 (1 + \xi/M_0)^2} \frac{\delta P(X,p;t)}{\delta X} \\
+ \quad & \beta \frac{p + \int \pi \psi'}{M_0(1 + \xi/M_0)} \int dx \phi_c' \Big(\psi'' - \psi U'(\Phi)\Big) - \frac{p + \int \pi \psi'}{(M_0 + \xi)^2} P(X,p;t) \\
+ \quad & \epsilon \frac{\delta}{\delta p}\Big[p P(X,p;t)\Big] + \frac{\epsilon}{\beta}\Big(\int \Phi'\Phi'\Big) \frac{\delta^2 P(X,p;t)}{\delta p^2} \Bigg\}\ . \qquad \text{(H.16)}
\end{aligned}
$$

Appendix I

Potentials and Masses for Kink-Antikink ϕ^4 Collisions

Since the analytic expressions for the potentials $V_i(x_0, y_0)$ and masses $m_i(x_0, y_0)$ in Chapter 7 are somewhat lengthy, we include them here, along with some useful properties and Taylor series. Since the integrals have already been published [15], we merely reproduce these analytic expressions, pointing out an error of 1/2 in the mass m_2. Since the "relativistic" calculations given involve integrals similar to those done by Campbell et al. [15], we recast the expressions in terms of three functions $w_i(\, z_0)$ with z_0 given by

$$z_0 \equiv \frac{m x_0 y_0}{\sqrt{2}\lambda} \ . \tag{I.1}$$

In terms of these functions w_i the potentials and masses take the form:

$$V_1 = \frac{\sqrt{2}m^3 y_0}{2\lambda}\left[\frac{4}{3} - w_1(z_0)\right] , \tag{I.2}$$

$$V_2 = \frac{\sqrt{2}m^3}{4\lambda y_0} w_2(z_0) \ , \tag{I.3}$$

$$m_1 = \frac{\sqrt{2}m^3 y_0}{\lambda}\left[\frac{4}{3} + w_1(z_0)\right] , \tag{I.4}$$

$$m_2 = \frac{\sqrt{2}m^3 x_0}{\lambda} w_1(z_0) \ , \tag{I.5}$$

$$m_3 = \frac{\sqrt{2}m^3}{4\lambda y_0} w_2(z_0) \ , \tag{I.6}$$

with the functions w_i given by

$$w_1(z_0) = \frac{\mathrm{sech}(z_0)(1+\tanh^2(z_0))}{\tanh^3(z_0)}\Big(z_0 - \frac{\tanh(z_0)}{1+\tanh^2(z_0)}\Big) \ , \tag{I.7}$$

$$
\begin{aligned}
w_2(z_0) &= \frac{16(1+\tanh^2(z_0))}{\tanh(z_0)}\Big(z_0 - \frac{\tanh(z_0)}{1+\tanh^2(z_0)}\Big) \\
&- \frac{8(1+\tanh^2(z_0))^2}{\tanh^2(z_0)}\Bigg[\Big(3 - \frac{4\tanh^2(z_0)}{1+\tanh^2(z_0)^2}\Big)z_0 - \frac{3\tanh(z_0)}{1+\tanh^2(z_0)}\Bigg] \\
&+ \frac{2(1+\tanh^2(z_0))^3}{\tanh^3(z_0)}\Bigg[\Big(5 - \frac{12\tanh^2(z_0)}{1+\tanh^2(z_0)^2}\Big)z_0 + \frac{16\tanh^3(z_0)}{3(1+\tanh^2(z_0)^3)} \\
&\qquad - \frac{5\tanh(z_0)}{1+\tanh^2(z_0)}\Bigg]\,, \qquad \text{(I.8)}
\end{aligned}
$$

$$
\begin{aligned}
w_3(z_0) &= \frac{1}{3}\left(\frac{\pi^2}{6} - 1\right) \\
&- \frac{2}{\sinh^2(2z_0)}\left[\frac{\pi^2}{12}\Big(\frac{2z_0}{\tanh(2z_0)} - 1\Big) - \frac{4z_0^3}{3\tanh(2z_0)}\right]\,. \qquad \text{(I.9)}
\end{aligned}
$$

With the aide of MACSYMA [136] the following Taylor series were computed:

$$
\begin{aligned}
w_1(z_0) &\approx \frac{4}{3} - \frac{32}{15}z_0^2 + \frac{128}{63}\,z_0^4 - \frac{1024}{675}\,z_0^6 \\
&+ \frac{2048}{2079}\,z_0^8 - \frac{11321344}{19348875}\,z_0^{10} + \frac{65536}{200475}\,z_0^{12}\,, \qquad \text{(I.10)}
\end{aligned}
$$

$$
\begin{aligned}
w_2(\,z_0) &\approx \frac{64}{3}\,z_0^2 - \frac{512}{15}\,z_0^3 + \frac{2816}{315}\,z_0^4 + \frac{2048}{189}\,z_0^5 \\
&- \frac{2048}{189}\,z_0^6 - \frac{16384}{1575}\,z_0^7 - \frac{421888}{51975}\,z_0^8 + \frac{32768}{6237}\,z_0^9 \\
&+ \frac{219250688}{42567525}\,z_0^{10} - \frac{181141504}{70945875}\,z_0^{11} + \frac{1906180096}{638512875}\,z_0^{12}\,, \qquad \text{(I.11)}
\end{aligned}
$$

$$
\begin{aligned}
w_3(\,z_0) &\approx \frac{4\pi^2}{45}\,z_0^2 + \frac{80\pi^2+336}{945}\,z_0^4 + \frac{896\pi^2+6400}{14175}z_0^6 - \frac{6400\pi^2+59136}{675}\,z_0^8 \\
&+ \frac{15566848\pi^2+167731200}{638512875}\,z_0^{10} - \frac{5218304\pi^2+62267392}{383107725}\,z_0^{12}\,. \qquad \text{(I.12)}
\end{aligned}
$$

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

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COLLECTIVE COORDINATES FOR NONLINEAR KLEIN-GORDON FIELD THEORIES

by

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Dedication

To my Mother

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