

# 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]

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

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

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

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

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

where we have taken  $\psi_0$  to be zero and introduced the following definitions

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

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

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  $\psi$  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  $\eta_\psi$ , and performed averages over the phonon degrees of freedom by assuming for the equilibrium distribution function for the phonons,

$$P_{eq} = e^{-\beta H_{ph}} , \quad (6.1.4)$$

with  $H_{ph}$  given by

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

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

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

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

which allows us to write

$$H_{ph} = \sum \omega_k |b_k|^2 . \quad (6.1.8)$$

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

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

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

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

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

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:

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

and

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

where

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

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

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

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

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

$$= \frac{T}{M_0}, \quad (6.1.17)$$

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

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

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

$$\equiv \alpha T^2. \quad (6.1.20)$$

In both sine-Gordon and  $\phi^4$  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  $\alpha$  is finite. Using these relations we find

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

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

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

where

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

$$= \frac{T}{M_0}, \quad (6.1.24)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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  $\Phi$ . This in turn leads via Eq. (B.10) of Appendix B to the following second-order equation of motion for  $X(t)$

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

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

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

has the correlation

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

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

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

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)

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

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

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

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

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

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  $\psi^3$ , 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  $\psi^3$  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  $\Phi$ , 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  $\Phi(x, t)$

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

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

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

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  $\Pi_0(x, t)$ :

$$\dot{\Phi} = \Pi_0 \quad (6.3.3)$$

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

where as before  $\Phi$  and  $\Pi_0$  are canonically conjugate variables. The standard form [108] for the bivariate functional Fokker-Planck equation is

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

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

$$A_{\Phi}[\Phi, \Pi_0] = \lim_{\Delta t \rightarrow 0} \frac{\langle \Delta\Phi \rangle}{\Delta t} , \quad (6.3.6)$$

$$A_{\Pi_0}[\Phi, \Pi_0] = \lim_{\Delta t \rightarrow 0} \frac{\langle \Delta\Pi_0 \rangle}{\Delta t} , \quad (6.3.7)$$

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

$$B_{\Phi\Pi_0}[\Phi, \Pi_0] = \lim_{\Delta t \rightarrow 0} \frac{\langle \Delta\Phi \Delta\Pi_0 \rangle}{\Delta t} , \quad (6.3.9)$$

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

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

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

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

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

with the Hamiltonian given by

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

which one would expect from equilibrium statistical mechanics. The most important aspect of this solution is evident when the Hamiltonian is written in terms of the new transformed variables  $X, p, \psi, \pi$

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

where

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

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

where the background field  $\psi_0$  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  $\psi$  field attains

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

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

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

we can rewrite the Hamiltonian as

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

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  $\psi$  field ( $\xi$  depends on  $\psi$  linearly) with a coefficient proportional to  $\dot{X}^2$ . This means that in doing the functional integral over  $\psi$  one must complete the square in the  $\psi$  variable, giving rise to a nonzero equilibrium value for  $\psi$  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  $\Phi$  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

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

where the functions  $H_n$  are Hermite polynomials and the  $\alpha_n$  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

$$p \int \pi \psi' \quad (6.3.21)$$

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 equilibrate much faster than the kink degrees of freedom, that is we make an adiabatic ansatz. The specific form of the ansatz is

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

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)

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

where

$$\mathcal{F}(x, t) \equiv F(x, t) - \frac{\phi'_c(x)}{M_0} \int \phi'_c(x - X) F(x, t), \quad (6.3.24)$$

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

$$\langle \mathcal{F}(x, t) \mathcal{F}(x', t') \rangle = 2T\epsilon \left[ \delta(x - x') - \frac{\phi'_c(x)\phi'_c(x')}{M_0} \right] \delta(t - t'), \quad (6.3.25)$$

$$= 2T\epsilon \delta_\psi(x - x') \delta(t - t'), \quad (6.3.26)$$

where the  $\delta_\psi$  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  $\psi$  field

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

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

This equation has an equilibrium solution

$$P^{eq} \equiv e^{-\beta H_{ph}} , \quad (6.3.28)$$

with  $H_{ph}$  given by

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

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

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

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  $\psi$  and  $\pi$  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  $\psi$  and  $\pi$  fields. Since  $H_{ph}$  is quadratic in the both

$\psi$  and  $\pi$ , all odd terms in either of these fields average to zero leaving us with

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

where here the angle brackets denote

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

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

$$\begin{aligned} &\int \phi'_c [\Phi'' - U'[\Phi]] \\ &= \int \phi'_c [\phi_c'' + \psi'' - U[\phi_c] - \psi U''[\phi_c] + O[\psi^2]] \end{aligned} \quad (6.3.33)$$

$$= \int \phi'_c [\psi'' - \psi U''[\phi_c]] + O[\psi^2] , \quad (6.3.34)$$

$$= \int [\phi'_c \psi'' - \psi \frac{d}{dx} U'[\phi_c]] + O[\psi^2] , \quad (6.3.35)$$

$$= \int [\phi'_c \psi'' + \psi' U'[\phi_c]] + O[\psi^2] , \quad (6.3.36)$$

$$= O[\psi^2] , \quad (6.3.37)$$

where we have made repeated use of

$$U'[\phi_c] = \phi_c'' . \quad (6.3.38)$$

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

$$T^2 p P(X, p; t) . \quad (6.3.39)$$

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

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

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]

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

Although this form for  $p$  still involves the field  $\psi$  (through  $\xi$ ), it does not depend on the momentum  $\pi$ . Compare this with the expression for  $p$  obtained from Eq. (3.3.28),

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

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  $\psi$ . 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

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

Again making the ansatz

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

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

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

where we have made use of the fact that

$$\int dx \Pi_0 \Phi' = p. \tag{6.3.46}$$

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

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

This is nearly identical with the result obtained in the previous section, the difference occurring 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  $X, p, \psi, \pi$  is conserved for all time because it satisfies 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

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

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

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

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

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

is a solution to Eq. (6.3.48). However, this Hamiltonian is unbounded from below due to the term linear in  $\Phi$  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  $\Phi_0$  given by

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

One of the obvious ways to account for this deviation is to use a nonzero  $\psi_0$  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  $\psi_0$  field, however since the kink will be moving (either at or approaching a terminal velocity),  $\psi_0$  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  $(2\pi)$ ). 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 expressible in terms of Jacobi elliptic 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  $2\pi$  ( $=0$ ) 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 beginning to the end of the kink can be less than  $2\pi$  [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.

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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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