Thermal corrections to overdamped soliton motion

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A singular perturbation theory is developed for evaluating the thermal effects on overdamped soliton motion. I find that the mobility of an overdamped sine-Gordon kink in the static limit is the same as given by Büttiker and Landauer and that the effect of an increase in the temperature is to increase this mobility by the factor $[1+(1.075...)/\beta E_0+\cdots]$, where E_0 is the rest energy of a kink. I also evaluate the change in the shape of an overdamped sine-Gordon kink caused by thermal fluctuations and find that the kink somewhat flattens, increasing its width.

I. INTRODUCTION

Recently there has been controversy^{1,2} concerning the relative validity of two different methods^{3,4} for calculating the current carried by a driven, heavily damped sine-Gordon chain. In one case, a hierarchy based on the Smolouchowski equation (SEH), is used and in the other case,⁴ principles from a nucleation theory (NT) are used. Neither method is exact and each one uses different approximations^{1,2} for obtaining their results. So it would be of value to have an exact analytic result against which these methods could be compared. The presentation of such a result is the purpose of this paper, as well as to demonstrate how singular perturbation theory can be applied to soliton systems in a temperature bath.

The critical difference between these two methods is best illustrated by their predicted values for the mobility of a single kink. If we use the notation of Büttiker and Landauer,⁴ then the overdamped equation of motion would be

$$\gamma \partial_t \theta = \kappa \partial_x^2 \theta - U(\theta) + F + \epsilon \zeta , \qquad (1)$$

where γ is the damping constant, κ is the torsion constant, $\int^{\theta} U d\theta$ is the retarding potential (whence -U is the torque), F is a spatially independent externally applied torque, and ζ is a thermal random torque. In Eq. (1), ϵ is an expansion parameter which we shall use later. For the overdamped sine-Gordon case, $U(\theta) = V_0 \sin \theta$, where V_0 is the strength of the retarding potential.

Let us now compare these theories. The NT takes and uses the zero-temperature mobility, which at zero torque⁴ is

 $\mu_{\rm NT} = \frac{\pi}{4\gamma} \left(\frac{\kappa}{V_0} \right)^{1/2},$

and then defines a current of $j = 2\pi\mu F(2n_0)$ where n_0 is the density of kinks. Although the SEH does not directly predict a mobility, it does predict a current. If we take its predicted value for the current and define a mobility from $\mu = j/2\pi F 2n_0$, then the SEH mobility would be

$$\mu_{\rm SEH} = (\beta E_0) \mu_{\rm NT} ,$$

where $\beta = (k_B T)^{-1}$ and E_0 is the energy of formation for a single kink. Thus the SEH value is singular as $T \rightarrow 0$. Since the only current carriers are the kinks and antikinks, the only way for the mobility to increase proportional to βE_0 as $T \rightarrow 0$ is for the kinks to move faster as $T \rightarrow 0$. At first this does not seem reasonable, and as we shall see here, such a behavior does not occur. However, let us also note that this singular nature in the mobility is not predicted by the SEH theory to exist all the way down to T=0, but only down to some relatively small value of T, which is inversely proportional to $\gamma^{2,3}$ But by choosing γ to be sufficiently large, one could make this critical value of T to be as small as desired. So one point which I want to look at is whether or not the mobility does behave as βE_0 for T greater than some relatively small value. I do not find such a behavior, but it must be mentioned that supporting this singular nature are computer simulations⁵ which give a best fit when one uses a factor of $(E_0\beta)^{3/2}$ instead of $E_0\beta$. However, the reliability of these simulations has been questioned.⁴

On the other hand, the zero-temperature value used in the NT theory seems to be more reasonable, since it has a constant value for the mobility as $T \rightarrow 0$. However, neither method is exact, and both methods depend on various approximations.^{1,2}

The value of the mobility in the limit of $T \rightarrow 0$, and for T small, is a quantity one would expect

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could be calculated by a perturbation theory. What is in question here is not the value at T=0, but rather the value as T approaches zero from above. So it is not sufficient to simply do the calculation at T=0, which has been done in Ref. 4. Rather, one must explicitly include the thermal fluctuations, perform the necessary averages, and then take the limit of $T \rightarrow 0$. In doing this calculation, one simplification occurs upon noting that in the limit of $T \rightarrow 0$, the density of kinks vanishes exponentially, so that kink-antikink and kink-kink collisions become less and less frequent. Thus we may consider the kinks to behave like free and noninteracting particles, and we may ignore that small time which is spent in collisions. So the problem can be reduced to considering a single simple kink moving under the influence of an external torque and a temperature bath.

However, this is still not as easy and straightforward as one might at first think it to be. For example, the most obvious approach would be expanding, e.g.,

 $\theta = \langle \theta \rangle + \delta \theta$,

where the angular brackets indicate an ensemble average and $\delta\theta$ is the deviation from the mean. Each element in this ensemble is determined by specifying the value of $\zeta(x,t)$. But this is wrong. Why this would be wrong may be seen by considering the motion in the position of a single kink, and by comparing its mean motion with the motion for a typical element from the ensemble. Owing to the thermal fluctuations, the center of the kink will execute a random walk, and for almost any element from the ensemble its position will move farther and farther away, as $t^{1/2}$, from its mean position for the mean motion. Thus whereas $\langle \theta \rangle$ will have a kink at some mean position, for a typical element from the ensemble, θ could have the kink at a considerable distance away (proportional to $t^{1/2}$), and thus $\delta\theta$, which is the difference between these two, can no longer be small even if the thermal fluctuations are small. A perturbation expansion based on this type of an expansion can only converge for t so small that the position of the kink for almost any element in the ensemble has not moved further than a distance on the order of its width.

The difficulty with the above expansion was that $\delta\theta$ was essentially the difference between two onelink solutions with the kinks at two different positions. If we would take this difference *after* translating the solutions until the two kinks more or less coincide, then we could expect $\delta\theta$ to remain small for all time. This is the idea in the following singular perturbation expansion. Take

$$\theta = \theta_0(x - x_0(t)) + \delta\theta(x, t)$$
,

where θ_0 will be a kink solution and $x_0(t)$ will be the position of the kink.⁶ For a given element from the ensemble, $x_0(t)$ can be uniquely determined, and shall be so determined such that the θ_0 term in the above expression will closely follow the actual kink, as it is being bounced back and forth by the random thermal fluctuations. As we shall see later, a perturbation theory based on the above type of an expansion will be convergent.

However, this will introduce several new features into the treatment of this problem which do deserve comment. First, one will note that we now have two statistical variables, $x_0(t)$ and $\delta\theta(x,t)$, instead of $\theta(x,t)$. Thus $\delta\theta$ must have exactly one less degree of freedom than θ has, and this will be achieved by requiring $\delta\theta$ to be orthogonal to the Goldstone mode. Further, this decomposition of θ into a kink variable x_0 and a continuum variable $\delta\theta$ will be seen to be a very natural decomposition, and is simply another reflection of the particlelike nature^{7,8} of the kink.

Another feature deserving comment is the definition of the ensemble averages. As an example, consider the ensemble average of $\theta(x,t)$ when given by the above expansion. The first term to be averaged is $\theta_0(x - x_0(t))$, requiring the average of a function of a statistical variable, not just the average of a statistical variable. Furthermore, since $x_0(t)$ will undergo a random walk, the ensemble average of $\theta_0(x - x_0(t))$ will also be time dependent, complicating the physical interpretation considerably. The source of this difficulty is again the act of trying to average solutions with kinks at different positions. The obvious way to bypass this is to define the ensemble average relative to the kink. As an example of what I mean by this, define $\chi = x - x_0(t)$, so that $\theta(x,t) = \theta_0(\chi) + \delta \theta$. Now average the first term by keeping χ the same for every element from the ensemble. Then it is clear that $\langle \theta_0(\chi) \rangle = \theta_0(\chi)$ since $\theta_0(\chi)$ is only a function and is not a statistical variable. All statistical variations have been swept into $\delta\theta$ by averaging relative to the center of the kink. Also, I wish to point out that the transformation from (x,t) coordinates into $[\chi = x - x_0(t), \tau = t]$ coordinates is a canonical transformation⁹ provided one appropriately defines the momentum. The quantity χ shall be referred to as the "comoving coordinate."

It is very easy to numerically evaluate ensemble averages at constant χ . As shall be seen shortly, given a definite element from the ensemble, there is a definite solution for $x_0(t)$. So as one is numerically solving for $\theta(x,t)$, one could also numerically solve for $x_0(t)$. Now by a simple translation one can transform the function $\theta(x,t)$ into the function $\theta(\chi,\tau)$, and then average this latter function.

In the next section I shall apply this singular per-

turbation expansion to a single kink in a temperature bath. The treatment shall be quite general, and I shall not specialize to the sine-Gordon case until in a-later section. First I shall expand the general solution out to second order in ζ (which will be first order in temperature), and it shall be clear that the expansion could be continued indefinitely without secular terms appearing. Then in Sec. III, I shall discuss the ensemble averaging of various variables at constant χ , from which one could evaluate the current.

The above results are valid for any value of the applied torque F, but not so high such that kinks will be spontaneously generated. However, their evaluation will require the knowledge of certain eigenstates as a function of F. These are not known in a closed form even for the sine-Gordon case. So in order that one may obtain analytic results, I will also treat the small-F case, expanding the above results in a regular perturbation expansion in F. Explicit results will be given for first order in F, and numerical values will be obtained for the terminal velocity of a kink for the sine-Gordon model and for the change in the shape of a kink when there is a nonzero temperature.

II. SINGULAR PERTURBATION EXPANSION

As discussed in the Introduction, I shall expand θ as

$$\theta(x,t) = \theta_0(\chi) + \epsilon \theta_1(\chi,\tau) + \epsilon^2 \theta_2(\chi,\tau) + \cdots , \qquad (2)$$

where ϵ is the expansion parameter, $\tau = t$, and χ is the comoving coordinate

$$\chi = x - \int_0^t v(t)dt .$$
 (3)

I shall also similarly expand the instantaneous velocity

$$v = v_0 + \epsilon v_1(t) + \epsilon^2 v_2(t) + \cdots, \qquad (4)$$

where v_0 is to be a constant, although the higher orders may be time dependent as indicated. Then inserting these equations into Eq. (1), expanding in powers of ϵ gives in zeroth order

$$-\kappa\theta_{0,\chi\chi} - \gamma v_0\theta_{0,\chi} + U(\theta_0) = F , \qquad (5)$$

in first order

$$\gamma \theta_{1,\tau} + L \theta_1 = \gamma v_1 \theta_{0,\chi} + \zeta , \qquad (6)$$

in second order

$$\gamma \theta_{2,\tau} + L \theta_2 = \gamma v_1 \theta_{1,\chi} + \gamma v_2 \theta_{0,\chi} - \frac{1}{2} U_{\theta\theta} \theta_1^2 , \qquad (7)$$

and so on. In the above, the operator L is

$$L = -\kappa \partial_{\chi}^2 - \gamma v_0 \partial_{\chi} + U_{\theta}(\theta_0) .$$
(8)

The operator L as well as Eq. (5) have been discussed in Ref. 1 for the sine-Gordon case. However, I am treating a more general case, so I must say a few words about the general properties of U and L.

I shall assume that Eq. (5) has a well-behaved solution corresponding to a single kink. By this I mean that θ_0 approaches the constant values of $\overline{\theta}_{\pm\infty}$ as $\chi \to \pm \infty$, determined by $U(\overline{\theta}_{\pm\infty}) = F$. Also, $\overline{\theta}_{+\infty}$ and $\overline{\theta}_{-\infty}$ are to differ by an amount appropriate for a kink (or antikink) solution. Also a unique value of v_0 is assumed to exist. Naturally, each of these parameters $\overline{\theta}_{\pm\infty}$ and v_0 are understood to be functions of the applied torque F.

One important feature of this zeroth-order solution is obtained upon differentiating (5) with respect to χ . One finds

$$L\left[\theta_{0,\chi}\right] = 0 , \qquad (9)$$

from whence it follows that the operator L has a zero eigenvalue, the Goldstone mode. I shall assume that there is only one such zero eigenvalue, and that all other eigenvalues have a positive real part. This assumption is made since a negative real part for the eigenvalue would correspond to an instability, as one could see from the left-hand side of Eq. (6). One example of such an instability is when the applied torque F is so large that kinks (or antikinks, depending on the sign of F) are spontaneously generated. (At this value of F, the continuous spectrum of L has just started to extend into negative real values.)

I shall also assume that $U_{\theta}(\theta)$ approaches the single value of $\kappa \eta^2$ as $\chi \to +\infty$ and as $\chi \to -\infty$. η has the dimensions of inverse length⁻¹, and will indicate the kink's width.

The continuous eigenstates of L are defined to be those solutions that approach the plane wave $e^{il\chi}$ as $\chi \rightarrow \pm \infty$, giving the continuous eigenvalues of L to be complex. These eigenvalues are

$$\lambda_l = \kappa l^2 - i\gamma v_0 l + \kappa \eta^2 , \qquad (10)$$

which is obtained from the eigenvalue problem

$$L\psi_l = \lambda_l \psi_l , \qquad (11)$$

by evaluating it at $\chi = \pm \infty$. Since this problem is non-Hermitian, I must use the adjoint states to define an inner product. The adjoint problem is

$$L^A \phi_l^A = \lambda_l \phi_l^A , \qquad (12)$$

where

$$L^{A} = -\kappa \partial_{\chi}^{2} + \gamma v_{0} \partial_{\chi} + U_{\theta}(\theta_{0}) . \qquad (13)$$

γ

I choose the ψ_l and ϕ_l^A states to be normalized so that

$$\langle \phi_l^A | \psi_{l'} \rangle = \delta(l - l') , \qquad (14)$$

where I shall now use the parentheses to indicate the inner product

$$\langle u | v \rangle \equiv \int_{-\infty}^{\infty} u(\chi) v(\chi) d\chi$$
 (15)

By prior assumption both L and L^A have one and only one bound state of zero eigenvalue, where

$$L\psi_b = 0 , \qquad (16)$$

$$L^A \phi_b^A = 0 . \tag{17}$$

These functions may be chosen to be normalized such that

$$\langle \phi_b^A | \psi_b \rangle = 1 , \qquad (18)$$

$$\langle \phi_b^A | \psi_l \rangle = 0 = \langle \phi_l^A | \psi_b \rangle . \tag{19}$$

I shall also assume that these eigenstates are complete.¹⁰ Then by (14), (18), and (19), the closure relation must be

$$\delta(\chi - \chi') = \phi_b^A(\chi')\psi_b(\chi) + \int_{-\infty}^{\infty} \phi_l^A(\chi')\psi_l(\chi)dl ,$$
(20)

where in (20) we have also assumed that the range of the continuous parameter l may be chosen to be exactly the same as is in the Schrödinger case. With the above, we may proceed to solve Eqs. (6) and (7) for the first- and second-order corrections due to the thermal fluctuations ζ .

In a singular perturbation expansion as I am doing here, one may (arbitrarily) demand that the fluctuations in θ always remain orthogonal to the bound-state component. This then determines v to all orders. To illustrate this, we take

$$\theta_1(\chi,\tau) = \int_{-\infty}^{\infty} \psi_l(\chi) f_{1l}(\tau) dl , \qquad (21)$$

and explicitly omit the $\lambda=0$ bound-state component. Next insert (21) into (6), and take the inner product of the result with ϕ_b^A . One then finds

$$\gamma v_1 = \frac{-1}{N} \langle \phi_b^A \, | \, \zeta \rangle \,\,, \tag{22}$$

$$N \equiv \langle \phi_b^A \mid \theta_{0\chi} \rangle , \qquad (23)$$

which uniquely determines v_1 . We remark that due to (9) and (17), and the assumption of only one $\lambda = 0$ bound state, $\theta_{0\chi}$ and ψ_b must be proportional. Thus due to (18), the term $N = \langle \phi_b^A | \theta_{0\chi} \rangle$ in (22) must be nonzero.

Next, from (6) and (21), upon taking the inner product with ϕ_l^A , one obtains

$$\partial_{\tau} f_{1l} + \lambda_l f_{1l} = \langle \phi_l^A | \xi \rangle , \qquad (24)$$

which will uniquely determine f_{1l} up to an initial condition. By prior assumption, the real part of λ_l is positive. Thus the homogeneous solution of (24) will exponentially vanish, and if the initial conditions were imposed at a very long time ago in the past, one has

$$f_{1l} = \int_{-\infty}^{\tau} \frac{d\tau'}{\gamma} \langle \phi_l^A | \zeta(\tau') \rangle \exp\left[-\frac{\lambda_l}{\gamma}(\tau - \tau')\right].$$
(25)

Now (21), (22), and (25) give the first-order solution.

The second-order solution follows similarly from Eq. (7). As before, I take

$$\theta_2(\chi,\tau) = \int_{-\infty}^{\infty} f_{2l}(\tau) \psi_l(\chi) dl$$
 (26)

and obtain

$$\gamma v_2 = \frac{1}{2N} \langle \phi_b^A \mid U_{\theta\theta} \mid \theta_1^2 \rangle - \frac{\gamma v_1}{N} \langle \phi_b^A \mid \theta_{1\chi} \rangle \quad (27)$$

and

$$f_{2l} = \int_{-\infty}^{\tau} d\tau' \left[v_1 \langle \phi_l^A | \theta_{1\chi} \rangle - \frac{1}{2\gamma} \langle \phi_l^A | U_{\theta\theta} | \theta_1^2 \rangle \right] \\ \times \exp\left[-\frac{\lambda_l}{\gamma} (\tau - \tau') \right], \qquad (28)$$

where the first set of large parentheses in (28) is understood to be evaluated at τ' .

It should also be clear by now that this type of expansion could be continued indefinitely, without secular terms appearing. This is guaranteed when the real part of λ_l is always positive. Now that we have a method for expanding the general solution, let us turn our attention to ensemble averages.

III. SECOND-ORDER ENSEMBLE AVERAGES

The solution in the preceding section is for a specific forcing term, $\zeta(x,t)$, from the ensemble. In general, we do not know which specific forcing term from the ensemble is driving the system, so we average over all elements in the ensemble to determine typical or average values. As is standard, I take¹

$$\begin{split} &\langle \zeta(x,t) \rangle_{\rm av} = 0 , \\ &\langle \zeta(x,t) \zeta(x',t') \rangle_{\rm av} = \frac{2\gamma}{\beta} \delta(x-x') \delta(t-t') , \end{split}$$

where now the angular brackets with the subscripts

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"av" indicate an ensemble average and $\beta = (k_B T)^{-1}$. Because the correlation time for the driving term is taken to be zero, one finds upon transforming into comoving coordinates that

$$\left\langle \zeta(\chi,\tau)\right\rangle_{\rm av} = 0 \tag{29}$$

and

$$\langle \zeta(\chi,\tau)\zeta(\chi',\tau')\rangle_{\rm av} = \frac{2\gamma}{\beta}\delta(\chi-\chi')\delta(\tau-\tau')$$
. (30)

Thus statistically speaking, the driving term in comoving coordinates is exactly the same as it is in laboratory coordinates (x,t). I should emphasize that this is true only as long as the correlation time remains zero.

As a consequence of (29), all first-order averages vanish. For the second-order averages, only the two quantities $\langle v_1\theta_1 \rangle_{av}$ and $\langle \theta_1^2 \rangle_{av}$ are required, as can be seen from Eqs. (27) and (28). Each of these may be readily evaluated by using (21), (22), (25), and (30), which give

$$\langle v_1 \theta_1 \rangle_{av} = \frac{-1}{\gamma \beta N} \int_{-\infty}^{\infty} dl \, \psi_l(\chi) \langle \phi_b^A \, | \, \phi_l^A \rangle , \qquad (31)$$

$$\langle \theta_1^2 \rangle_{\rm av} = \frac{2}{\beta} \int_{-\infty}^{\infty} dl \psi_l(\chi) \int_{-\infty}^{\infty} dl' \psi_{l'}(\chi) \frac{\langle \psi_{l'} | \psi_{l'} \rangle}{\lambda_l + \lambda_{l'}} \,.$$
(32)

We note that due to closure, Eq. (20), the above expression for $\langle v_1 \theta_1 \rangle_{av}$ reduces to

$$\langle v_1 \theta_1 \rangle_{av} = \frac{1}{\gamma \beta N} \left[\psi_b(\chi) \langle \phi_b^A | \phi_b^A \rangle - \phi_b^A(\chi) \right] .$$
(33)

Thus one only needs to know the bound state in order to evaluate this ensemble average.

The evaluation of (32) is more difficult. One could use the analytic properties of the eigenfunctions to eliminate one of the l integrals by distorting the contour into the upper half-plane. But then the remaining l integral will contain a square-root radical, which prevents a closed-form evaluation. Nevertheless, this would be a convenient form for numerical evaluation since it involves a single l integral and not a double integral.

However, the emphasis here is not on numerical evaluation, but on analytic results. So next I shall take the $F \rightarrow 0$ limit and demonstrate how to proceed in this limit.

IV. WEAK TORQUE LIMIT

Now I shall proceed to expand the previous results for F small. I shall introduce superscripts to

designate the order in F, e.g.,

$$\theta_0 = \theta_0^{(0)} + \theta_0^{(1)} F + \theta_0^{(2)} F^2 + \cdots$$
 (34)

I shall also assume that in the absence of any torque, the kink's velocity is zero, whence $v_0^{(0)} = 0 = v_2^{(0)}$, etc. Then when Eq. (5) is expanded, we find

$$-\kappa\theta_{0\chi\chi}^{(0)} + U(\theta_0^{(0)}) = 0 , \qquad (35)$$

$$L^{(0)}\theta_0^{(1)} = \gamma v_0^{(1)}\theta_{0\chi}^{(0)} + 1 , \qquad (36a)$$

$$L^{(0)}\theta_0^{(2)} = \gamma v_0^{(1)}\theta_{0\chi}^{(1)} + \gamma v_0^{(2)}\theta_{0\chi}^{(0)} - \frac{1}{2}U_{\theta\theta}(\theta_0^{(1)})^2 ,$$

(36b)

where

$$L^{(0)} = -\kappa \partial_{\chi}^{2} + U_{\theta}(\theta_{0}^{(0)}) .$$
(37)

As before, Eq. (36a) yields

$$\gamma v_0^{(1)} = \frac{-1}{N^{(0)}} \langle \phi_b^{(0)} | 1 \rangle , \qquad (38)$$

$$\theta_0^{(1)} = \int_{-\infty}^{\infty} dk \frac{1}{\lambda_k^{(0)}} \psi_k^{(0)} \langle \phi_k^{(0)} | 1 \rangle , \qquad (39)$$

where the superscript zeros refer to the appropriate zero-torque quantities. One will note that the superscripts A have been deleted from $\phi_k^{(0)}$ and $\phi_b^{(0)}$ since $L^{(0)}$ is now self-adjoint. Also, we may now normalize $\phi_b^{(0)}$ and $\psi_b^{(0)}$ so that $\phi_b^{(0)} = \psi_b^{(0)}$, whence $\langle \phi_b^{(0)} | \phi_b^{(0)} \rangle = 1$. The list of the remaining important first order in F quantities follows:

$$\psi_b^{(1)} \!=\! - \int_{-\infty}^{\infty} dk rac{\psi_k^{(0)}}{\lambda_k^{(0)}} \langle \phi_k^{(0)} | L^{(1)} \psi_b^{(0)}
angle \, ,$$

(40b)

$$\phi_b^{A(1)} = -\int_{-\infty}^{\infty} dk \frac{\phi_k^{(0)}}{\lambda_k^{(0)}} \langle \psi_k^{(0)} | L^{A(1)} \phi_b^{(0)} \rangle ,$$

$$N^{(1)} = \int_{-\infty}^{\infty} dk \frac{1}{\lambda_{k}^{(0)}} \langle \phi_{b}^{(0)} | \partial_{\chi} \psi_{k}^{(0)} \rangle \langle \phi_{k}^{(0)} | 1 \rangle , \qquad (41)$$

$$\psi_{k}^{(1)} = \frac{1}{\lambda_{k}^{(0)}} \psi_{b}^{(0)} \langle \phi_{b}^{(0)} | L^{(1)} \psi_{k}^{(0)} \rangle$$

+ $\mathscr{P} \int_{-\infty}^{\infty} dl \frac{\psi_{l}^{(0)}}{\lambda_{k}^{(0)} - \lambda_{l}^{(0)}}$
 $\times \langle \phi_{l}^{0} | (L^{(1)} - \lambda_{k}^{(1)}) \psi_{k}^{(0)} \rangle , \quad (42a)$

$$\begin{split} \phi_{k}^{A(1)} &= \frac{\phi_{b}^{(0)}}{\lambda_{k}^{(0)}} \langle \psi_{b}^{(0)} | L^{A(1)} \phi_{k}^{(0)} \rangle \\ &+ \mathscr{P} \int_{-\infty}^{\infty} dl \frac{\phi_{l}^{(0)}}{\lambda_{k}^{(0)} - \lambda_{l}^{(0)}} \\ &\times \langle \psi_{l}^{(0)} | (L^{A(1)} - \lambda_{k}^{(1)}) \phi_{k}^{(0)} \rangle , \end{split}$$
(42b)

where in (42), \mathscr{P} indicates the Cauchy principal value and

$$L^{(1)} = -\gamma v_0^{(1)} \partial_{\chi} + U_{\theta\theta} \theta_0^{(1)} , \qquad (43a)$$

$$L^{A(1)} = +\gamma v_0^{(1)} \partial_{\chi} + U_{\theta\theta} \theta_0^{(1)} , \qquad (43b)$$

$$\lambda_{k}^{(1)} = -i\gamma v_{0}^{(1)}k \ . \tag{44}$$

Using these results, one may expand $\langle v_1 \theta_1 \rangle_{av}$ and $\langle \theta_1^2 \rangle_{av}$ in a power series of F. First from (33),

$$\langle v_1 \theta_1 \rangle_{\rm av}^{(0)} = 0$$
, (45a)

$$\langle v_1 \theta_1 \rangle_{\rm av}^{(1)} = \frac{1}{\gamma \beta N^{(0)}} (\psi_b^{(1)} - \phi_b^{A^{(1)}}) ,$$
 (45b)

etc. Expansion of $\langle \theta_1^2 \rangle_{av}$ is not so simple, but there are some tricks for reducing the complexity. For example, the inner product $\langle \phi_l^{(0)} | \phi_l^{(0)} \rangle$ can be simplified. Since $L^{(0)}$ is self-adjoint, it follows that the adjoint eigenfunctions must be some linear combination of the $L^{(0)}$ eigenfunctions. Thus

$$\phi_l^{(0)} = a_l \psi_{-l}^{(0)} + b_l \psi_l^{(0)} . \tag{46}$$

Then it follows that

$$\langle \phi_{l'}^{(0)} | \phi_{l}^{(0)} \rangle = a_l \delta(l'+l) + b_l \delta(l-l')$$
 (47)

Thus when f_l is even in l, but otherwise arbitrary, we find

$$\int_{-\infty}^{\infty} dl \,\psi_l^{(0)} f_l \langle \phi_{l'}^{(0)} \,|\, \phi_l^{(0)} \rangle = f_{l'} \phi_{l'}^{(0)} \,. \tag{48}$$

With the use of these results an expansion of (32) then yields

$$\langle \theta_{1}^{2} \rangle_{av}^{(0)} = \frac{1}{\beta} \int_{-\infty}^{\infty} dl \frac{1}{\lambda_{l}^{(0)}} \psi_{l}^{(0)} \phi_{l}^{(0)} ,$$

$$\langle \theta_{1}^{2} \rangle_{av}^{(1)} = \frac{1}{\beta} \int_{-\infty}^{\infty} dl \frac{1}{\lambda_{l}^{(0)}} \left[2\phi_{l}^{(0)} \psi_{l}^{(1)} - \frac{\lambda_{l}^{(1)}}{\lambda_{l}^{(0)}} b_{l} \psi_{l}^{(0)} \psi_{l}^{(0)} \right.$$

$$+ 4\mathscr{P} \int_{-\infty}^{\infty} dl' \frac{\lambda_{l}^{(0)} \psi_{l}^{(0)} \psi_{l}^{(0)}}{(\lambda_{l}^{(0)} + \lambda_{l'}^{(0)})(\lambda_{l}^{(0)} - \lambda_{l'}^{(0)})} \langle \phi_{l'}^{(0)} | (L^{A(1)} - \lambda_{l}^{(1)}) \phi_{l}^{(0)} \rangle \right] .$$

$$(49)$$

Now from (27), an expansion of $\langle v_2 \rangle_{av}$ yields

$$\langle v_{2} \rangle_{av}^{(0)} = 0 ,$$

$$\gamma N^{(0)} \langle v_{2} \rangle_{av}^{(1)} = \frac{1}{2} \langle \phi_{b}^{A(1)} | U_{\theta\theta} \langle \theta_{1}^{2} \rangle_{av}^{(0)} \rangle + \frac{1}{2} \langle \phi_{b}^{(0)} | U_{\theta\theta\theta} \theta_{0}^{(1)} \langle \theta_{1}^{2} \rangle_{av}^{(0)} \rangle - \gamma \langle \phi_{b}^{(0)} | \partial_{\chi} \langle v_{1} \theta_{1} \rangle_{av}^{(1)} \rangle$$

$$+ \frac{1}{2} \langle \phi_{b}^{(0)} | U_{\theta\theta} \langle \theta_{1}^{2} \rangle_{av}^{(1)} \rangle .$$
(50a)
$$(50a) = 0 ,$$

$$(50a) = 0 ,$$

$$+ \frac{1}{2} \langle \phi_{b}^{(0)} | U_{\theta\theta} \langle \theta_{1}^{2} \rangle_{av}^{(1)} \rangle .$$

$$(50b) = 0 ,$$

$$(50a) = 0 ,$$

$$+ \frac{1}{2} \langle \phi_{b}^{(0)} | U_{\theta\theta} \langle \theta_{1}^{2} \rangle_{av}^{(1)} \rangle .$$

There are two more relationships which can give further simplifications. The first one arises upon differentiating (36a), whence one finds

$$\frac{1}{N^{(0)}}L^{(0)}\theta_{0\chi}^{(1)} + U_{\theta\theta}\theta_{0}^{(1)}\phi_{b}^{(0)} = \gamma v_{0}^{(1)}\partial_{\chi}\phi_{b}^{(0)}$$

and thus

$$\langle \psi_{k}^{(0)} | L^{A(1)} \phi_{b}^{(0)} \rangle = 2\gamma v_{0}^{(1)} \langle \psi_{k}^{(0)} | \partial_{\chi} \phi_{b}^{(0)} \rangle - \frac{1}{N^{(0)}} \lambda_{k}^{(0)} \langle \psi_{k}^{(0)} | \partial_{\chi} \theta_{0}^{(1)} \rangle , \qquad (51a)$$

$$\langle \phi_{k}^{(0)} | L^{(1)} \psi_{b}^{(0)} \rangle = -\frac{1}{N^{(0)}} \lambda_{k}^{(0)} \langle \phi_{k}^{(0)} | \partial_{\chi} \theta_{0}^{(1)} \rangle .$$
(51b)

The other is a similar identity which can simplify the calculations involved in evaluating $\langle v_2 \rangle_{av}^{(1)}$. This is

$$\phi_{b}^{(0)}U_{\theta\theta}\psi_{k}^{(0)}\psi_{l}^{(0)} = \frac{\lambda_{k}^{(0)} - \lambda_{l}^{(0)}}{2N^{(0)}}(\psi_{k\chi}^{(0)}\psi_{l}^{(0)} - \psi_{l\chi}^{(0)}\psi_{k}^{(0)}) + \frac{1}{N^{(0)}}\partial_{\chi}[(U_{\theta} - \frac{1}{2}\lambda_{k}^{(0)} - \frac{1}{2}\lambda_{l}^{(0)})\psi_{k}^{(0)}\psi_{l}^{(0)} - \kappa\psi_{k\chi}^{(0)}\psi_{l\chi}^{(0)}] .$$
(52)

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Proceeding any further would be best done with a model. In the next section I shall evaluate $\langle v_2 \rangle_{av}^{(1)}$ and $\langle \theta_2 \rangle_{av}^{(0)}$ for the sine-Gordon model.

V. RESULTS FOR THE SINE-GORDON MODEL

For this model one takes

$$U = \kappa \eta^2 \sin \theta , \qquad (53)$$

and upon solving for the zeroth-order solution one obtains

$$\theta_0^{(0)} = 4 \tan^{-1}(se^z) , \qquad (54)$$

where s = +1 for a kink, -1 for an antikink, and $z = \eta \chi$. Thus

$$\theta_{0,\chi}^{(0)} = \frac{2s\eta}{\cosh z} , \qquad (55a)$$

$$\sin\theta_0^{(0)} = -2s \frac{\sinh z}{\cosh^2 z} , \qquad (55b)$$

$$\cos\theta_0^{(0)} = 1 - \frac{2}{\cosh^2 z}$$
, (55c)

$$U_{\theta\theta}(\theta_0^{(0)}) = \kappa \eta^2 2s \frac{\sinh z}{\cosh^2 z} , \qquad (55d)$$

and the eigenfunctions are⁷

$$\phi_b^{(0)} = \psi_b^{(0)} = \left(\frac{\eta}{2}\right)^{1/2} \operatorname{sech} z$$
, (56a)

$$\psi_{k}^{(0)} = \frac{e^{ik\chi}(k+i\eta \tanh z)}{[2\pi(k^{2}+\eta^{2})]^{1/2}} , \qquad (56b)$$

$$\phi_k^{(0)} = -\psi_{-k}^{(0)} = \frac{e^{ik\chi}(k - i\eta \tanh z)}{[2(k^2 + \eta^2)]^{1/2}} , \qquad (56c)$$

where

$$\lambda_k^{(0)} = \kappa(\eta^2 + k^2) \tag{57}$$

and $b_k = 0$ [see Eq. (49)]. From (23), (38), and the above, we find

$$N^{(0)} = 2s (2\eta)^{1/2} , \qquad (58)$$

$$v_0^{(1)} = -\frac{s\pi}{4\gamma\eta} \ . \tag{59}$$

It becomes convenient to define the function

$$g(z,z') = \int_{-\infty}^{\infty} dk \frac{1}{\lambda_k^{(0)}} \phi_k^{(0)}(\chi') \psi_k^{(0)}(\chi) , \qquad (60)$$

which for the sine-Gordon model is

$$g(z,z') = \frac{\frac{1}{2}e^{-2z} + \frac{1}{2}e^{2z} - |z-z'|}{4\kappa\eta \cosh z \cosh z'}, \qquad (61)$$

where $z_{>}(z_{<})$ is the greater (lesser) of $z = \eta \chi$ and $z' = \eta \chi'$. Then

$$\langle \theta_1^2 \rangle_{\rm av}^{(0)} = \frac{1}{\beta} g(z,z) = \frac{2 - {\rm sech}^2 z}{4\kappa \eta \beta} , \qquad (62a)$$

$$\theta_0^{(1)} = \frac{1}{\eta} \int_{-\infty}^{\infty} dz' g(z, z') .$$
 (62b)

In the following calculations, certain integrals will frequently occur. These and their values are

$$\int_{-\infty}^{\infty} dz' \frac{g(z,z')}{\cosh z'} = 0 , \qquad (63a)$$

$$\int_{-\infty}^{\infty} dz' \frac{g(z,z')}{\cosh^3 z'} = \frac{1 - \ln(2\cosh z)}{3\kappa\eta \cosh z} , \qquad (63b)$$

$$\int_{-\infty}^{\infty} dz' \frac{g(z,z')}{\cosh^5 z'} = \frac{2 + \operatorname{sech}^2 z - \frac{8}{3} \ln(2 \cosh z)}{10 \kappa \eta \cosh z} ,$$
(62a)

$$\int_{-\infty}^{\infty} \frac{dz'}{\cosh z'} \partial_{z'} g(z,z') = \frac{z}{2\kappa\eta \cosh z} , \qquad (63d)$$

$$\int_{-\infty}^{\infty} \frac{dz'}{\cosh^3 z'} \partial_{z'} g(z,z') = \frac{\sinh z}{4\kappa\eta \cosh^2 z} (3 + \operatorname{sech}^2 z) ,$$

$$\int_{-\infty}^{\infty} dz' \frac{z' \sinh z'}{\cosh^4 z'} g(z, z') = \frac{5 + 6z \tanh z - 8 \ln(2 \cosh z)}{24\kappa\eta \cosh z} . \quad (63f)$$

For evaluating $\langle v_2 \rangle_{av}$ from (50), it is now simply a matter of evaluating the various matrix elements in (51). I find

$$\langle \phi_b^{A(1)} | U_{\theta\theta} \langle \theta_1^2 \rangle_{av}^{(0)} \rangle = \frac{\pi}{4\beta\kappa\eta^2} \left(\frac{38}{15} \ln 2 - \frac{13}{6} \right) \left(\frac{\eta}{2} \right)^{1/2},$$
(64a)

$$\langle \phi_b^{(0)} | U_{\theta\theta\theta} \theta_0^{(1)} \langle \theta^2 \rangle_{av}^{(0)} \rangle$$

$$= \frac{\pi}{4\beta\kappa\eta^2} \left(\frac{\gamma}{6} - \frac{34}{15}\ln^2\right) \left[\frac{\eta}{2}\right]^{1/2}, \quad (64b)$$

$$\langle \phi_b^{(0)} | \partial_\chi \langle v_1 \theta_1 \rangle_{\mathrm{av}}^{(1)} \rangle = \frac{\pi}{16\beta\kappa\gamma\eta^2} \left[\frac{\eta}{2} \right]^{1/2}.$$
 (64c)

The last matrix element in (50b) is the worst to calculate. This I shall do in sections. With the use of the identity (52), all gradient terms integrate to zero, leaving

$$\langle \phi_{b}^{(0)} | U_{\theta\theta} \langle \theta_{1}^{2} \rangle_{av}^{(1)} \rangle = \frac{2}{\beta N^{(0)}} \int_{-\infty}^{\infty} dl \frac{1}{\lambda_{l}(0)} \langle \phi_{l,\chi}^{(0)} | (L^{(1)} - \lambda_{l}^{(1)}) \psi_{l}^{(0)} \rangle$$

$$+ \frac{2}{\beta N^{(0)}} \int_{-\infty}^{\infty} dl \int_{-\infty}^{\infty} dl' \frac{1}{\lambda_{l}^{(0)} + \lambda_{l'}^{(0)}} \langle \phi_{l'}^{(0)} | (L^{A(1)} - \lambda_{l}^{(1)}) \phi_{l}^{(0)} \rangle$$

$$\times (\langle \psi_{l'}^{(0)} | \partial_{\chi} \psi_{l}^{(0)} \rangle - \langle \psi_{l}^{(0)} | \partial_{\chi} \psi_{l'}^{(0)} \rangle) .$$
(65)

This is then evaluated to be

$$\langle \phi_b^{(0)} | U_{\theta\theta} \langle \theta_1^2 \rangle_{\text{av}}^{(1)} \rangle$$

$$= \frac{\pi}{8\beta\kappa\eta^2} (1 - \frac{8}{15}\ln 2 - J) \left[\frac{\eta}{2}\right]^{1/2}, \quad (66)$$

where

$$J = 2\pi \int_0^\infty \frac{dv}{\sinh^2(\pi v)} \left[1 - \frac{1}{(1+v^2)^{1/2}} \right]$$

= 0.149 409 4..., (67)

with the numerical value being obtained from a Hewlett-Packard HP41CV calculator, using the simple trapezoid rule. Setting all of the above together gives the very simple value

$$\langle v_2 \rangle_{\rm av}^{(1)} = -s \frac{\pi (1 + \frac{1}{2}J)}{32\beta\gamma\kappa\eta^2} . \tag{68}$$

Thus to this order, the average velocity of a kink or an antikink shall be

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$$v = -\frac{s\pi F}{4\gamma\eta} \left[1 + \frac{1 + \frac{1}{2}J}{\beta E_0} + \cdots \right] + \cdots , \qquad (69)$$

where $E_0 = 8\kappa\eta$ and is the rest energy of a single kink. Equation (69) shows that the effect of an increase in the temperature is to increase the velocity.

This is as one would expect in that the thermal fluctuations allow the damped kinks to move faster.

As a final calculation, I shall determine the change in the shape of a kink due to temperature fluctuations. For this calculation, I shall take the F=0 limit. From (26), (28), (45), and (49), one determines that

$$\langle \theta_2 \rangle_{\rm av}^{(0)} = -\frac{s}{4\beta} \int_{-\infty}^{\infty} dz' (2 \operatorname{sech} z' - \frac{1}{3} \operatorname{sech}^3 z') \\ \times \partial_{z'} g(z, z') ,$$

which evaluates to

$$\langle \theta_2 \rangle_{\rm av}^{(0)} = \frac{-s}{4\beta\kappa\eta} ({\rm sech}z)$$

 $\times [z - \frac{1}{4} {\rm tanh}z (1 + \frac{1}{3} {\rm sech}^2 z)].$ (70)

Thus to this order

$$\theta = 4 \tan^{-1} (se^z) + \langle \theta_2 \rangle_{av}^{(0)} + \cdots , \qquad (71)$$

and the effect of an increase in the temperature is to flatten out the kink, thus increasing its width.

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adding to the understanding, I shall assume these bound states to be absent. One could account for these

additional bound states by applying the general rule of

replacing all integrals over l by an integral *plus* a sum over the additional bound states.