Overdamped soliton motion

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The problem of finding the current carried by the driven, heavily damped, sine-Gordon chain has been solved by two methods. Trullinger *et al.* [Phys. Rev. Lett. 40, 206, 1603(E) (1978)] and Guyer and Miller [Phys. Rev. A 17, 1774 (1978)] have employed an approximate treatment of the hierarchy of equations generated by the Smolouchowski equation (the SEH method) to calculate the current analytically and numerically. Büttiker and Landauer [Phys. Rev. Lett. 43, 1453 (1979); and (unpublished)] have criticized this treatment and have proposed an alternate treatment employing ideas from nucleation theory (the NT method). These two methods of solution are reviewed and compared. Both methods are shown to involve the same ansatz for the nonequilibrium probability distribution function. The SEH method employs an exact integration of the steady-state one-particle current equation; the NT method employs an approximate integration of the steady-state nucleation current equation. The approximations underlying the use of the two methods are described. Criticism of the SEH method by Büttiker and Landauer is discussed.

I. INTRODUCTION

Over the past several years there has been considerable effort in the development of the theory of the statistical mechanics of nonlinear systems. This effort has arisen in part because of the challenge offered by this conceptually difficult problem and because of the experimental investigations of systems that are able to be modeled by nonlinear equations, i.e., systems with important properties that probe nonlinearity.[1] The equilibrium statistical mechanics of simple nonlinear systems (e.g., the ϕ^4 chain, the sine-Gordon chain, etc.) are well understood. Much less well understood is the theory of the dynamics of nonlinear systems. This is in part because of the variety of system conditions that can influence one's judgement as to the basic elements that must be incorporated in a theory of the dynamics. (For example the system may contain a dilute, weakly interacting, thermally generated soliton-antisoliton gas or a dense, heavily damped, "pressure" and thermally generated soliton "gas," etc.) It is also in part because some of the analytic methods are new and have yet to stand the test of time.

The dynamics of heavily damped nonlinear systems have been the subject of several papers and some discussion. Trullinger *et al.*[2] (I6) and Guyer and Miller[3] have described the heavily damped sine-Gordon chain in an external field using the Smolouchowski equation (SE). Because they were interested in the case of a strongly interacting system in an external field of arbitrary strength, these authors employed a method of solution that leaned heavily on the similarity of the basic equations to those encountered in the description of dense fluids. This method is called the Smolouchowski equation hierarchy method, SEH method, and variations on it have proven particularly useful in the development of a general formalism for treating the dynamics of nonlinear systems in the heavy damping limit.[4–6] Landauer, in a series of private communications[7] and in collaboration with Büttiker,[8] has proposed an alternative method for treating the "driven sine-Gordon chain" that is based on nucleation theory,[9] NT. In addition Landauer[7] and Landauer and Büttiker[8] have criticized the method employed by I6 and Guyer and Miller in principle and with respect to certain details.

The purpose of this paper is to discuss the description of the dynamics of the heavily damped sine-Gordon chain in an external field (determination of the rate of phase evolution) with an emphasis on exposing the similarities and differences of the various approaches, and on indicating the elements of a correct theory. We find, and the discussion below is oriented toward making this point, that the method of solution employed by I6 and Guyer and Miller, the SEH method, is in principle much the same as that advocated by Büttiker and Landauer, the nucleation theory method. However, the SEH method involves exact integration of equations in contrast with the approximate NT treatment. Further by being embedded in a systematic hierarchical apparatus, the SEH method lends itself much more readily to improvement and generalization. In Secs. II and III we look at a simple-model problem to illustrate the SEH and NT methods. We examine a number of important

general properties of the behavior of the Smolouchowski equation in Sec. IV and we review a number of features of the SEH method with an eye toward understanding its relationship to the NT method. In Sec. V, we critically examine the assumptions which form the basis of the NT method and in Sec. VI we review our findings and discuss the essential content of the two theories.

II. MODEL PROBLEM

Here and in Sec. III we look at a model problem using the SEH and the NT method. The idea is to see the essential features of the methods in a context that is simple and does not obscure what is going on with superfluous detail.

Consider a pair of particles, 1 and 2, that form a molecule, held together by a spring, that resides in a region of space containing a sinusoidal potential. The Hamiltonian of the system is $E=p^2/2I+V(12)$, where I is the moment of inertia of the particles and

$$V(12)=-E_1(\cos\theta_1+\cos\theta_2)+\tfrac{1}{2}E_2(\theta_2-\theta_1)^2 \ , \quad (1)$$

$\theta_i=2x_i/a$. The particles in the molecule are subject to the constant external force F, $V_e(12)=-F(\theta_1+\theta_2)$ and are sufficiently damped by the medium in which they reside that the distribution function describing the pair is the Smolouchowski equation for diffusion through configuration space

$$\frac{\partial\sigma(12)}{\partial t}+\vec{\nabla}_2\cdot\vec{J}(12)=0 \ , \quad (2)$$

where $\vec{\nabla}_2=(\partial/\partial 1,\partial/\partial 2)$ and

$$J_1(12)=\frac{1}{\tau}\left[\frac{\partial\sigma(12)}{\partial 1}+\frac{\partial\beta U(12)}{\partial 1}\sigma(12)\right] \ , \quad (3)$$

$$J_2(12)=\frac{1}{\tau}\left[\frac{\partial\sigma(12)}{\partial 2}+\frac{\partial\beta U(12)}{\partial 2}\sigma(12)\right] \ , \quad (4)$$

where $\tau=\beta I\eta$, η is the coefficient of viscosity, and $U(12)=V(12)+V_e(12)$. Here 1 stands for θ_1, etc., $\sigma(12)$ is the probability distribution function, and $J_1(12)$ and $J_2(12)$ are the probability current components in the directions 1 and 2 of configuration space, respectively (see Fig. 1). In thermal equilibrium $F=0$, the solution to Eq. (2) is

$$\sigma(12)=\rho(12)=\exp[-\beta V(12)].$$

In addition $J_1(12)=J_2(12)=0$; the probability current in configuration space is *pointwise* zero. When $F\neq 0[V_e(12)\neq 0]$ the molecule is driven at a constant rate by the field: a steady state results. This steady state is described completely by the behavior of the probability current in configuration space: $\vec{\nabla}_2\cdot\vec{J}=0$. It can also be described *approximately* by statements about the behavior of the averaged probability currents in configuration space. For example:

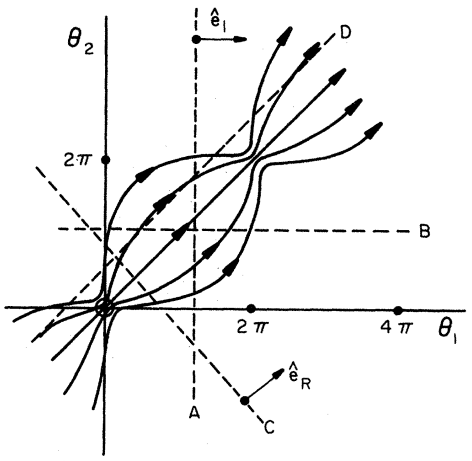

FIG. 1. Currents and configuration space. To calculate the rate of phase evolution for particle 1, one projects $\vec{J}$ onto $\hat{e}_1$ ($\hat{e}_1$ is a unit vector in the 1 direction) and integrates over the surface A. The result is the net probability current from $\theta_1=0$ to 2π. Formally this procedure is equivalent to $\int d1\cdots dN\delta(\hat{e}_1\cdot\vec{u})\hat{e}_1\cdot\vec{J}(1\cdots N)$. The net center-of-mass current passes through the surface C, etc. Note: the relative current is not pointwise zero; it is zero at any r when integrated over all R.

(a) The probability current in the $\hat{1}$ direction is constant

$$J_1(1)\equiv\int d2\,J_1(12)=\text{const}\equiv\bar{J} \ , \quad (5)$$

or the equivalent statement

$$J_2(2)\equiv\int d1\,J_2(12)=\bar{J} \ . \quad (6)$$

(b) The averaged probability current in the center-of-mass direction, $\hat{e}_R=(1,1)/\sqrt{2}$, is constant,

$$J_R(R)=\int dr\,J_R(Rr)=\bar{J} \ , \quad (7)$$

where

$$J_R(Rr)=[J_1(12)+J_2(12)]/\sqrt{2} \ ,$$

$$R=(\theta_1+\theta_2)/2 \ ,$$

and

$$r=\theta_2-\theta_1 \ .$$

[The constants on the right-hand side of Eqs. (5)–(7) are the same since the individual particles move in steady state at the same rate as the center of mass.]

(c) The averaged probability current in the relative

motion direction, $\hat{e}_r = (1,-1)/\sqrt{2}$, is zero

$$J_r(r) = \int dR\, J_r(Rr) = 0 \quad , \tag{8}$$

where

$$J_r(Rr) = [J_1(12) - J_2(12)]/\sqrt{2} \quad .$$

The probability current for relative motion, $J_r(Rr)$, need not be pointwise zero but it is zero when averaged over all R because the forces at work on the molecule do not lead to a net rate of motion of its constituents relative to one another; the molecule does not come apart (see Fig. 1).

Equations (5)–(8), equations for certain average probability currents, amount to truncated differential equations for the probability distribution function, $\sigma(12)$, see below. These equations can be used to advantage in analyzing approximate solutions to the full steady-state Smolouchowski equation, $\vec{\nabla}_2 \cdot \vec{J} = 0$.

Let us consider an example of the use of Eqs. (5)–(8) to solve $\vec{\nabla}_2 \cdot \vec{J} = 0$ in an approximate way. Since $\rho(12)$ solves $\vec{\nabla}_2 \cdot \vec{J} = 0$ exactly when $F = 0$, we seek a solution to Eq. (2) in the form $\sigma(12) = \rho(12)e(12)$. Then from Eqs. (5)–(8)

$$J_r(Rr) = \rho(12)\left[\frac{\partial e(Rr)}{\partial R} + \beta F e(Rr)\right] \quad , \tag{9}$$

and

$$J_r(Rr) = \sqrt{2}\rho(12)\frac{\partial e(Rr)}{\partial r} \quad . \tag{10}$$

Equations (9) and (10) are exact. Now suppose that we choose to approximate $e(12)$ by a product ansatz

$$e(12) = E(R)e(r) \quad . \tag{11}$$

Then, the use of this ansatz in Eqs. (7) and (9) leads to

$$\bar{J} = \sigma(R)\left[\frac{\partial \hat{W}(R)}{\partial R} + \beta F\right] \quad , \tag{12}$$

where

$$\sigma(R) = \int dr\, \rho(Rr)E(R)e(r)$$

is the probabiltiy distribution function for the center of mass and $E(R) \equiv \exp \hat{W}(R)$. (Let us pause for a moment to remark on notation. The discussion will involve a variety of distribution functions that differ from one another in detail according to the manipulation being undertaken. We exhibit the notation we will use in Table I: ρ refers to uncorrected distribution function, $\hat{}$ denotes that the external field is incorporated into the distribution function. In some contexts this notation serves no useful purpose and we do not use it.) Equation (12) is an example of what we called a "truncated" differential equation above. Similarly, the use of this ansatz, Eq. (11), in

TABLE I. Notation for distribution functions, V denotes the equilibrium interaction potential, $\exp W$ is the modification of $\rho(\hat{\rho})$ to yield $\sigma(\hat{\sigma})$, $\exp \beta FR$ is due to the applied field.

$\rho = \exp(-\beta V)$
$\hat{\rho} = \exp(-\beta V + \beta FR)$
$\sigma = \exp(-\beta V + W(R)$
$\hat{\sigma} = \exp[-\beta V + W(R) + \beta FR] = \exp[-\beta V + \hat{W}(R)]$

Eqs. (10) and (8) leads to

$$0 = \sigma(r)\frac{\partial u(r)}{\partial r} \quad , \tag{13}$$

where

$$\sigma(r) = \int dR\, \rho(Rr)E(R)e(r)$$

is the probability distribution function for relative motion and $e(r) \equiv \exp u(r)$. From Eq. (13) we conclude that $u(r)$ must be zero. Then, Eq. (12) takes a simple form and can be solved by known methods. Define $W(R)$, $W(R) = \hat{W}(R) - \beta FR$, so that Eq. (12) becomes

$$\bar{J} = \hat{\sigma}(R)\frac{\partial W(R)}{\partial R} \quad , \tag{14}$$

where

$$\hat{\sigma}(R) \equiv \rho(R)\exp(+\beta FR)\exp W(R) \quad .$$

Integrate this center-of-mass differential equation on R and subject the solution to two constraints:

normalization:

$$\int_0^{2\pi} \hat{\sigma}(R)\, dR = 1 \quad , \tag{15}$$

periodicity:

$$\hat{\sigma}(R + 2\pi) = \hat{\sigma}(R) \quad . \tag{16}$$

The first of these constraints is a choice of normalization for $\hat{\sigma}(R)$ and the second follows from translational invariance of $V(12)$. Thus upon integration of Eq. (14) we obtain

$$W(2\pi) - W(0) = \bar{J}\int_0^{2\pi} dR\, \frac{1}{\hat{\sigma}(R)} \quad . \tag{17}$$

Now $\hat{\sigma}(2\pi) = \hat{\sigma}(0)$, $-\beta F 2\pi + W(2\pi) = W(0)$, or $W(2\pi) - W(0) = +\beta F 2\pi$ so that we have

$$\bar{J} = \beta F 2\pi \Big/ \int_0^{2\pi} \frac{dR}{\hat{\sigma}(R)} \quad . \tag{18}$$

With this equation, we have a solution for J (steady-state, center-of-mass probability current), using the SEH method. This solution is not exact since it uses

a $\sigma(12)$ that does not solve $\vec{\nabla}_2 \cdot \vec{J} = 0$ exactly; rather it is faithful to the statements about the averaged probability currents contained in items (b) and (c) above. In addition we had to fix an integration constant by appeal to physical argument.

III. NUCLEATION THEORY DESCRIPTION OF THE MODEL

As an alternative to the simple version of the SEH method described above, we might proceed quite differently. We are interested in the rate of molecule motion. This rate is related to the steady-state probability current $J_R(R)$. The steady-state probabililty current is *independent* of R and can thus be calculated at any R. It might be relatively easy to calculate this probability current by focusing only on local configurations which can cause evolution of the molecule through the 'ducts," the improbably occupied regions of configuration space, that connect two relatively probable configurations. For example from Eq. (1), with $F=0$, we see that for motion of the molecule from near $R=0$ to near $R=2\pi$ the duct is at $(R=\pi,\ r=0)$ where the potential energy has the form shown in Fig. 2. For $F\neq 0$ the duct remains at $r=0$ and is shifted along the R axis to $R(F)$, $(4\pi/a)E_1 \sin R(F) + F = 0$. (We have assumed the spring holds the molecule more or less intact as it is driven over the sinusoidal potential so that only one duct is of importance ; see Fig. 2 for an illustration of a more complex situation.) We will take the averaged steady-state probability current $J_R(R)$ to be the probability current that passes through the duct. This is given by Eq. (9):

$$J_R(Rr) = \rho(12)\left[\frac{\partial e(Rr)}{\partial R} + \beta F e(Rr)\right] .$$

As above we take $e(Rr)$ to have the form

$$e(Rr) = e^{\hat{W}(R) - \beta F R} \tag{19}$$

so that $J_R(Rr)$ becomes

$$J_R(Rr) = \hat{\sigma}(12)\frac{\partial \hat{W}(R)}{\partial R} . \tag{20}$$

Now, from Eq. (14), the steady-state probability current we seek is

$$\bar{J} = J_R(R) = \hat{\sigma}(R)\frac{\partial \hat{W}(R)}{\partial R} . \tag{21}$$

We will attempt to learn $\bar{J}$ by integrating Eq. (21) near the duct. To this end we must (a) locate the duct and (b) specify the behavior of $\hat{\sigma}(12)$ near the duct.

(a) The duct is taken to be located at the extremum $\hat{\rho}(12)$ [really $V(12)+V_e(R)$]; i.e., at $(\bar{R},\bar{r})$

$$\frac{4\pi}{a}E_1 \sin\bar{R} + F = 0 \tag{22}$$

and

$$\bar{r} = 0 . \tag{23}$$

(b) The behavior of the energy *near* the duct is given by

$$V(12) + V_e(12) = E_0 + \tfrac{1}{2}A_r r^2 - \tfrac{1}{2}A_R \delta R^2 , \tag{24}$$

where

$$E_0 = F\bar{R} + E_1 \cos\bar{R} , \quad A_r = E_2 = \frac{E_1}{2}(1-Q^2)^{1/2} ,$$

and

$$A_r = E_1(1-Q^2)^{1/2} ;$$

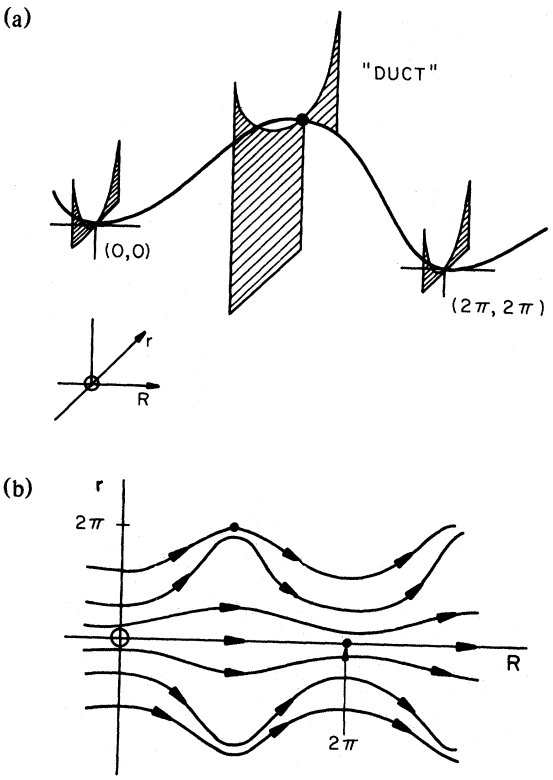

FIG. 2. "Duct" and probability current flow. (a) The probability current flow is primarily limited by a single "duct" in configuration space between two relatively probable configurations. When this is the case the probability current can be described near the "duct" with reasonable certainty. (b) There are situations in which more than one "duct" contributes importantly to the current from $R=0$ to 2π. If the spring E_2 is soft the molecule can move one "atom" at a time, then, there is a substantial current through "ducts" near $r=0$, near $r=\pm 2\pi$, etc.

$Q = F/2E_1$. Equations (22)–(24) are the information about the behavior of $\hat{\rho}(Rr)$ near the duct that will permit integration of Eq. (21). Use of Eq. (24) in Eq. (21) leads to

$$\bar{J} = \int dr\, e^{-\beta E_0} e^{-A_r r^2/2} e^{A_R \delta R^2/2} \frac{\partial e^{W(\bar{R}+\delta R)}}{\partial(\delta R)}$$

$$= \hat{\rho}(\delta R) \frac{\partial e^{W(\delta R)}}{\partial(\delta R)}$$

and

$$e^{W(\delta R >> 0)} - e^{W(\delta R << 0)} = \bar{J} \int \frac{d(\delta R)}{\hat{\rho}(\delta R)} \quad , \tag{25}$$

where

$$\hat{\rho}(\delta R) = e^{-\beta E_0} \left(\frac{2\pi}{A_r} \right)^{1/2} \exp \tfrac{1}{2}(A_R \delta R^2) \quad .$$

Carrying out the δR integration leads to

$$\bar{J} = \frac{(e^{W(\delta R >> 0)} - e^{W(\delta R << 0)})}{\int d(\delta R)/\hat{\rho}(\delta R)} = (\cdots) e^{-\beta E_0} \left(\frac{A_R}{A_r} \right)^{1/2} \quad . \tag{26}$$

To complete the specification of $\bar{J}$, we now need to know the behavior of W far from $\bar{R}$. A variety of arguments are given that permit $W(\delta R >> 0)$ and $W(\delta R << 0)$ to be specified in terms of known properties of the system. These arguments are of the same genre as the normalization and periodicity conditions that were used on Eq. (17). Thus in Eq. (26) we have a solution for $\bar{J}$, the steady-state, center-of-mass probability current. It is the nucleation theory equivalent of Eq. (18).

The two calculation procedures outlined here are very similar. We have exhibited some details of both that expose this similarity They both involve calculation of the steady-state, center-of-mass probability current using the ansatz $\sigma(12) = \rho(12)E(R)$. They differ in that the SEH method employs an exact treatment of the consequences of this ansatz where—as the NT method makes several approximations in handling this ansatz. Thus we expect the SEH method to give the "correct" result in places where they differ appreciably. Indeed, simply determining a procedure for locating the duct [finding the extremum of $V(12) + V_e(12)$ as in item (a), above Eq. (22)] introduces strong limitations on the region of validity of the NT method. That is, for the purpose of locating the duct and integrating Eq. (21) we want the extremum of $\bar{\sigma}(\bar{R})$, $\hat{\sigma}(R) = \hat{\rho}(R) \times \exp W(R)$. We, following BL (Büttiker and Landauer), take this to be given by the extremum of $\hat{\rho}(R)$, Eq. (22). This procedure is acceptable if $W(R)$ is small or slowly varying near the duct found from $\hat{\rho}(R)$. However, $W(R)$ is of order FR [see, e.g., Eqs. (17) and (18)]. Thus the procedure we have used for finding the duct is strictly correct only at $F \to 0$. Thus, to permit FR in $\hat{\rho}(R)$ to influence the location of the duct, while $W(R)$ is ignored, is inconsistent and leads to errors of order FR in the location of the duct.

IV. SMOLOUCHOWSKI EQUATION HIERARCHY

In this section we describe the SEH method of solution of the driven, heavily damped, sine-Gordon chain. The problem is described in detail in Guyer and Miller[3] as is the application of the SEH method. We will not dwell upon the details of the method here but rather we will indicate the important features of the calculational scheme together with any approximations used in making them. We shall also describe those features of the SEH method that permit one to treat the approximate solution of I6 and Guyer and Miller as the first step in a systematic and tractable scheme for solving the N-body SE. We review the SEH method as applied to the sine-Gordon chain: an N-particle problem. The N-particle sG chain is described by the potential energy

$$V(1 \cdots N) = -\sum_i E_1 \cos\theta_i + \frac{E_2}{2} \sum_i (\theta_{i+1} - \theta_i)^2 \tag{27}$$

in the external field

$$V_e(1 \cdots N) = -E_0 \sum_i \theta_i \quad . \tag{28}$$

The N-particle probability distribution function obeys the SE

$$\frac{\partial \sigma(1 \cdots N)}{\partial t} + \sum_{i=1}^{N} \frac{\partial}{\partial i} J_i(1 \cdots N) = 0 \quad , \tag{29}$$

where

$$J_i(1 \cdots N) = \frac{1}{\tau} \left(\frac{\partial}{\partial i} \sigma(1 \cdots N) + \sigma(1 \cdots N) \frac{\partial \beta U(1 \cdots N)}{\partial i} \right) \quad , \tag{30}$$

and $U = V + V_e$. It is useful to have available the equations of motion for the low-order probability distribution functions since it is these functions which are related to important physical quantities. We define

$$\sigma(1 \cdots n) = \int d(n+1) \cdots dN\, \sigma(1 \cdots N)$$

(neglecting an unimportant normalization). We find a hierarchy of equations for $\sigma(1)$, $\sigma(12)$, . . . , upon integration of Eq. (30) on $2 \cdots N$, $3 \cdots N$, etc:

$$\frac{\partial \sigma(1)}{\partial t} + \frac{\partial J_1(1)}{\partial 1} = 0 \quad , \tag{31}$$

$$\frac{\partial \sigma(12)}{\partial t} + \frac{\partial J_1(12)}{\partial 1} + \frac{\partial J_2(12)}{\partial 2} = 0 \quad , \tag{32}$$

$$\frac{\partial \sigma(1 \cdots N)}{\partial t} + \sum_i \frac{\partial J_i(1 \cdots N)}{\partial i} = 0 \quad , \tag{32'}$$

where

$$J_1(1)=\frac{1}{\tau}\left[\rho(1)\left(\frac{\partial e(1)}{\partial 1}+e(1)\frac{\partial\beta V_e(1)}{\partial 1}\right)+\sum_{j\neq(1)}\int dj\,\rho(1j)[e(1j)-e(1)]\frac{\partial\beta V(1j)}{\partial 1}\right] , \tag{33}$$

$$J_1(12)=\frac{1}{\tau}\left[\rho(12)\left(\frac{\partial e(12)}{\partial 1}+e(12)\frac{\partial\beta V_e(1)}{\partial 1}\right)+\sum_{j\neq(1,2)}\int dj\,\rho(12j)[e(12j)-e(12)]\frac{\partial\beta V(1j)}{\partial 1}\right] , \tag{34}$$

$$J_i(1\cdots N)=\frac{1}{\tau}\rho(1\cdots N)\left(\frac{\partial e(1\cdots N)}{\partial i}+\frac{\partial\beta V_e}{\partial i}e(1\cdots N)\right) . \tag{34'}$$

In writing Eqs. (33) and (34), we have used the Born-Bogoliubov-Green-Kirkwood-Yvon (BBGKY) equations for the n-particle *equilibrium* distribution functions $\rho(1)$, $\rho(12)$, . . . and the *definitions* $\sigma(1)\equiv\rho(1)e(1)$, $\sigma(12)\equiv\rho(12)e(12)$, for each $\sigma(1\cdots n)$. [The similarity of the structure of the equations for $J_1(1)$, $J_1(12)$, . . . to the corresponding equilibrium BBGKY equations[10] has led to the SEH method being referred to as the BBGKY "approximation."[7] This terminology is unfortunate.] Equations (31) and (32) are exact since they represent a collection of relations among defined quantities. In preparation for testing a number of approximate treatments of these equations we consider $J_R(12)$ and $J_r(12)$. These probability currents are constructed from $J_1(12)$ and $J_2(12)$ as described above. By the argument below Eq. (7) we have

$$J_R(R)=\int dr\,J_R(12)=J_1(1) .$$

For $J_r(12)$ we have

$$J_r(R,r)=\frac{1}{\sqrt{2}}[J_1(12)-J_2(12)] . \tag{35}$$

Using the indistinguishability of the motion of 1 relative to 2 from the motion of 2 relative to 1 we have

$$J_r(R,r)=(1/\sqrt{2})[J_1(21)-J_2(21)]=-J_r(Rr)$$

and $J_2(12)=J_1(21)$. Thus for $J_r(Rr)$ we find

$$J_r(Rr)=\sqrt{2}\rho(12)\frac{\partial e(12)}{\partial r} . \tag{36}$$

This equation is as simple in form as Eq. (10) above although it describes a remarkably more complicated system; $e(12)$ is sensitive to the fact that 1 and 2 are embedded in the middle of a chain.

In contradistinction to the theory of classical fluids, we shall direct our attention to the N-particle equations, (32') and (34') by introducing and discussing several approximate forms for $e(1\cdots N)$.

Ansatz 1. We choose $e(1\cdots N)$ to be in the (Hartree-like) form

$$e(1\cdots N)=h(1)h(2)\cdots h(N) . \tag{37}$$

Upon making the defintion $h(1)=e^{w(1)}$ we see that $\sigma(1\cdots N)$ has the analytic structure that permits $\sigma(1)$, $\sigma(12)$, . . . to be calculated directly in terms of the unknown pseudoexternal field, w, using transfer-integral techniques.[2-4] [We can also calculate $e(1)$, $e(12)$, . . . , of Eqs. (33) and (34) directly.] Note: Eq. (37) does *not* mean that $e(1)=h(1)$, $e(12)=h(1)h(2)$, . . . , . Using $w(1)$ then, Eq. (31) takes the form

$$\bar{J}=J_1(1)=\frac{1}{\tau}\sigma(1)\left(\frac{\partial w(1)}{\partial 1}+\beta F\right) , \tag{38}$$

where $\sigma(1)$ is a function of w determined exactly by solving a transfer-integral problem. We can now use the constraints equivalent to Eqs. (15) and (16) to obtain

$$\bar{J}\tau=\beta F 2\pi\Big/\int_0^{2\pi}\frac{d1}{\sigma(1)} . \tag{39}$$

It is important to note for practical purposes that the determination of $\sigma(1)$ for use in Eq. (39) involves the self-consistent determination of $w(1)$.

The ansatz in Eq. (37), used by I6 and Guyer and Miller, yields a form for $e(12)$ [$e(12)$ is symmetric in the interchange of 1 and 2] that does not in general satisfy $J_r(r)=0$. It is this failure that leads to the next level of approximation to $\sigma(1\cdots N)$; see ansatz 2 below.

The procedure carried out here is an example of the SEH method: (i) an approximate form to $\sigma(1\cdots N)$ is chosen that permits calculations of $\sigma(1)$, $\sigma(12)$, . . . ; (ii) the unknown functional forms in $\sigma(1\cdots N)$ are determined by appeal to the sequence of reduced Smolouchowski equations, Eqs. (31) and (32).

Ansatz 2. We choose $e(1\cdots N)$ to be of the form

$$e(1\cdots N)=h(1)h(2)\cdots h(N)\times f(12)f(23)\cdots f(N-1N) \tag{40}$$

and we define $h(1)=\exp w(1)$ and $f(12)=\exp u(12)$, and $u(12)=u(|x_1-x_2|)$. The constraint set by the steady-state single-particle probability current is the same as above [only $\sigma(1)$ is more complicated]

$$\bar{J}=\frac{1}{\tau}\sigma(1)\left[\frac{\partial w(1)}{\partial 1}+\beta F\right] . \tag{41}$$

The constraint $J_r(r)=0$ is not automatically satisfied, and constitutes the "equation of motion" for $u(r)$.

Ansatz 3. In general one proceeds by using approximate forms for $e(1\cdots N)$ that permit reasonably easy determination of the reduced n-particle distribution functions; i.e., that reduce the determination to a tractable transfer-integral problem. Then, a suitable number of current equations must be integrated in order to fix the unknown functions. In this manner we proceed to construct a systematic solution to the SE.

V. NUCLEATION THEORY

In this section we describe the NT approach to the driven, heavily damped, sine-Gordon chain problem. For the details of this method see Ref. 8. Below we shall indicate the important features of the NT scheme together with the approximations needed for its implementation. In order to make a comparison with the detailed treatment of BL more accessible we adopt their continuum version of the sine-Gordon chain.

Consider a continuum sine-Gordon chain described by the potential energy

$$E[\theta(x)]=\int\frac{dx}{a}\left[-E_1\cos\theta(x)+\frac{E_2a^2}{2}\left(\frac{\partial\theta}{\partial x}\right)^2-E_0\theta(x)\right] , \tag{42}$$

where configurations of the chain are given by $\theta(x)$ and the external field appears in Eq. (42). The equilibrium probability distribution function $\rho[\theta(x)]$, is a functional of $\theta(x)$. For $E_0\neq 0$ the probability distribution function $\sigma[\theta(x)]$ obeys the Smolouchowski equation

$$\frac{\partial\sigma[\theta(x)]}{\partial t}+\int\frac{dx}{a}\frac{\delta}{\delta\theta(x)}J(x;[\theta(x)])=0 , \tag{43}$$

where

$$J(x;[\theta(x)])=\frac{1}{\tau}\left[\frac{\delta}{\delta\theta(x)}\sigma[\theta(x)]+\sigma[\theta(x)]\frac{\delta\beta E[\theta(x)]}{\delta\theta(x)}\right] . \tag{44}$$

Equations (43) and (44) are the continuum version of Eqs. (29) and (30). We seek to solve Eq. (44) for the steady-state probability current using the ansatz

$$\hat{\sigma}[\theta(x)]=\exp\left[\int\frac{dx}{a}w[\theta(x)]\right]\hat{\rho}[\theta(x)] , \tag{45}$$

where

$$\hat{\rho}[\theta(x)]=\exp\{-\beta E[\theta(x)]\} .$$

This equation is the continuum version of ansatz 1 above, Eq. (37); the functional $\exp\{\int(dx/a)\times w[\theta(x)]\}$ is denoted by $\beta[\theta(x)]$ in Eq. (4.7) of BL. Substitution of Eq. (45) into Eq. (44) leads to

$$J(x;[\theta(x)])=\frac{1}{\tau}\hat{\sigma}[\theta(x)]\frac{\delta w[\theta(x)]}{\delta\theta(x)} , \tag{46}$$

the continuum version of Eq. (34'). (Note a minor difference associated with the use of ρ in the discrete chain problem instead of the $\hat{\rho}$ used here, the βF term, see Table I.)

Büttiker and Landauer argue that the steady evolution of phase arises under appropriate circumstances as a consequence of the soliton-antisoliton creation process (a nucleation process). Therefore the steady-state phase current, $\langle\partial\theta/\partial t\rangle$, the steady-state single-particle probability current, $\bar{J}$, and the steady-state nucleation current [a current through the duct in configuration space that connects the no soliton chain (0) to the chain with a soliton-antisoliton pair, $(S\bar{S})$] are all related to one another. BL establish a relationship between the steady-state nucleation current and the steady-state phase current. They then calculate the steady-state nucleation current. In a calculation of the steady-state nucleation current attention is focused on the region of configuration space near the duct that connects (0) to $(S\bar{S})$ (see Fig. 3). The center of the duct is located at a "suitable extremum" of $E[\theta(x)]$, $\bar{\theta}(x)$, and $E[\theta(x)]$ is then expanded about $\bar{\theta}(x)$ in terms of the normal modes of the chain about $\bar{\theta}(x)$, $\delta\psi_\nu(x)$. $E(\bar{\theta}(x))\equiv E[\theta(x)]_{\bar{\theta}}$ near the center of the duct can now be expressed as a function of the normal-mode amplitudes $\eta_0,\eta_1,\ldots$, and

$$E\left[\bar{\theta}(x)+\sum_\nu\eta_\nu\delta\psi_\nu(x)\right]=E(\bar{\theta}(x);\eta_0\eta_1\cdots)=E_0+\tfrac{1}{2}\sum e_\nu\eta_\nu^2 . \tag{47}$$

The "suitable extremum" called for here is a saddle-point configuration at which the energy is unstable to the motion described by the mode denoted

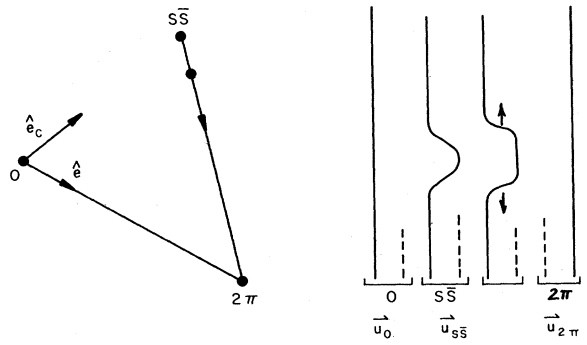

FIG. 3. Configuration space. The nucleation current flows from 0 to $S\bar{S}$, where 0 denotes the unkinked chain, $\vec{u}_0$, and $S\bar{S}$ denotes the kink-antikink chain, $\vec{u}_{S\bar{S}}$, at or near the critical nucleus. The probability current from 0 to $S\bar{S}$ [proportional to $\vec{J}\cdot\hat{e}_c$, $\hat{e}_c=(\vec{u}_{S\bar{S}}-\vec{u}_0)/|\vec{u}_{S\bar{S}}-\vec{u}_0|$] is a measure of the pair nucleation rate. The flow of probability from 0 to 2π (from $\vec{u}_0$ to $\vec{u}_{2\pi}$) is related to this rate.

by amplitude η_0. Evolution of the chain from (0) to $(S\bar{S})$ can now be described by evolution of η_0 from $\eta_0<0$ towards $\eta_0>0$, see Fig. 3.

$$\frac{\partial\hat{\sigma}(\bar{\theta}(x);\eta_0\eta_1\cdots)}{\partial t}+\sum_\nu\frac{\partial}{\partial\eta_\nu}j_\nu(\bar{\theta}(x);\eta_0\eta_1\cdots)=0\ , \tag{48}$$

where

$$j_\nu(\bar{\theta}(x);\eta_0\eta_1\cdots)=\frac{1}{\tau}\left[\frac{\partial\hat{\sigma}(\hat{\theta}(x);\eta_0\eta_1\cdots)}{\partial\eta_\nu}+\beta e_\nu\eta_\nu\sigma(\bar{\theta}(x);\eta_0\eta_1\cdots)\right]\ . \tag{49}$$

The parabolic approximation used for E in Eq. (49) will be valid in the neighborhood of the saddle point. The probability distribution function (near the duct) is taken to be given by Eq. (45)

$$\hat{\sigma}(\bar{\theta}(x);\eta_0\eta_1\cdots)=e^{W(\eta_0\eta_1\cdots)}\ \hat{\rho}(\bar{\theta}(x);\eta_0\eta_1\cdots)\ , \tag{50}$$

where

$$W(\eta_0\eta_1\cdots)=\int\frac{dx}{a}w\left[\bar{\theta}(x)+\sum_\nu\eta_\nu\delta\psi_\nu(x)\right] \tag{51}$$

and

$$\hat{\rho}(\theta(x);\eta_0\eta_1\cdots)=\exp[-\beta E(\bar{\theta}(x);\eta_0\eta_1\cdots)]\ .$$

Substitution of Eq. (50) in Eq. (49) leads to

$$j_\nu(\bar{\theta}(x);\eta_0\eta_1\cdots)=\frac{1}{\tau}\frac{\partial W(\eta_0\eta_1\cdots)}{\partial\eta_\nu}\times\hat{\rho}(\bar{\theta}(x);\eta_0\eta_1\cdots)\ . \tag{52}$$

The probability currents j_ν are not pointwise zero but like $J_r(Rr)$ in Sec. II they are expected to be zero on average near the duct (the single exception is j_0 which is nonzero on average). To make further progress we must assume $W(\eta_0\eta_1\cdots)$ to depend only on η_0 as $W(\eta_0)$. [BL find $W(\eta_0\eta_1\cdots)=W(\eta_0)$ by setting the currents j_ν identically to zero. This is merely an assumption.] Thus the ansatz for $\hat{\sigma}(\bar{\theta}(x);\eta_0\eta_1\cdots)$ employed by BL is not that of Eq. (45) as it appears in Eq. (50); it is

$$\hat{\sigma}(\bar{\theta}(x);\eta_0\eta_1\cdots)=e^{W(\eta_0)}\ \hat{\rho}(\bar{\theta}(x);\eta_0\eta_1\cdots)\ . \tag{53}$$

With this ansatz Eq. (49) for the probability current in the η_0 direction is

$$\bar{J}_0(\bar{\theta}(x);\eta_0\eta_1\cdots)=\frac{1}{\tau}\frac{\partial e^{W(\eta_0)}}{\partial\eta_0}\hat{\rho}(\bar{\theta}(x);\eta_0\eta_1\cdots)\ . \tag{54}$$

We integrate this equation on $\eta_1,\eta_2,\ldots$ to get the steady-state nucleation current $\bar{J}_0$,

$$\bar{J}_0=\frac{1}{\tau}\frac{\partial e^{W(\eta_0)}}{\partial\eta_0}\hat{\rho}(\bar{\theta}(x);\eta_0)\ . \tag{55}$$

Following the standard prescription (see Sec. II) this equation may now be integrated with respect to η_0 to yield

$$\bar{J}_0\tau=(e^{W(\eta_0>>0)}-e^{W(\eta_0<<0)})\Big/\int\frac{d\eta_0}{\hat{\rho}(\bar{\theta}(x);\eta_0)}\ . \tag{56}$$

As a final step $\exp W(\eta_0>>0)$ and $\exp W(\eta_0<<0)$ are specified. It is argued that $W(\eta_0>>0)\to-\infty$ and that $W(\eta_0<<0)$ is determined by requiring that the ansatz in Eq. (53) conforms to one's expectation about $\sigma[\theta(x)]$ near (0). The statement that $W(\eta_0>>0)\to-\infty$ means that the soliton pair must be driven apart by the field and acquire energy during one collision time that is large compared to k_BT; BL translate this into $\beta F>>m_0$, where m_0 is the soliton density.

Of course Eq. (56), achieved using the NT method, is superficially the same as Eq. (39), achieved using the SEH method. But is the physical content the same? The answer is in principle yes. Both methods involve the same ansatz for the probability distribution function. Both methods involve integration of a steady-state probability current equation. The integration procedures differ in the choice

of direction in which to project the current and in the choice of variables to be used in describing the relevant region of configuration space. It is the choice of implementation which distinguishes the two methods. In the SEH method, configuration space is described by $12\cdots N$ and the integration procedure involves variables $2\cdots N$ so that the steady-state probability current equation, Eq. (38), becomes an equation for the behavior of the probabiltiy distribution function of 1. Integration of this equation yields the steady-state probability current. Formally

$$\bar{J}_1(1)=\int d1\cdots N\delta(\vec{u}\cdot\hat{e})\hat{e}\cdot\vec{J}(1\cdots N)\ ,$$

where $\vec{u}=(u_1,u_2,\ldots,u_N)$ and $\hat{e}=(1,0,0,\ldots)$. In the NT method, configuration space is described by $\eta_0\eta_1\eta_2\cdots$ and the integration procedure involves variables $\eta_1\eta_2\cdots$ so that the steady-state probability current equation, Eq. (54), becomes an equation for the behavior of the probability distribution function of η_0. Integration of this equation yields the steady-state nucleation current. Formally

$$\bar{J}_0=\int d1\cdots N\delta(\vec{u}\cdot\hat{e})\hat{e}\cdot\vec{J}(1\cdots N)\ ,$$

where

$$\hat{e}=(\vec{u}_{S\bar{S}}-\vec{u}_0)/|\vec{u}_{S\bar{S}}-\vec{u}_0|$$

is a unit vector pointing from 0 to $S\bar{S}$ (here $\vec{u}_{S\bar{S}}$ is a configuration of the chain corresponding to a soliton pair at or beyond the critical nucleus and $\vec{u}_0$ is a configuration of the chain with no soliton pair, see Fig. 3). [$\delta(\vec{u}\cdot\hat{e})$ defines the surface in configuration space orthogonal to the direction of the current being calculated, orthogonal to $\hat{e}$.] The currents $\bar{J}_0$ and $\bar{J}_1$ are related as described by BL.

VI. DISCUSSION

In this section we summarize and compare the content of the two methods of solution of the driven, overdamped sine-Gordon chain.

1. The SEH method of solution is based on the belief that the system being described is a strongly interacting system possibly driven far from equilibrium. Thus the SEH method is designed to work at all fields and temperatures—it is not a perturbation approach. The ansatz of the low-order SEH method, Eq. (37), builds up the nonequilibrium distribution function from the equilibrium distribution function by a modification of the single-particle structure of the N-particle distribution function that is consistent with the existence of a steady-state current. The equilibrium distribution functions, $\rho(12)$, $\rho(123),\ldots,$ describe pairs, triples, etc., of particles that already reside in an inhomogeneous space with strongly correlated motions. The modification of the single-particle structure (for all particles) leads in turn to a modification of the correlated motion of pairs, triples, etc.

2. The hierarchy of equations that are generated from the Smolouchowski equation, the SEH, provide a tractable sequence of equations that can be employed for the systematic solution of the driven, sine-Gordon chain (or any similar problem). A possible scheme for improvement of the extent solution is suggested in Sec. II.

3. The current-field characteristic reported by I6 and Guyer and Miller are the results of exact (numerical) integration of the relevant equations.

4. Guyer and Miller reported an "activation energy" for kink or soliton creation as a function of the external field. As decribed by Guyer and Miller this "activation energy" was determined by analysis of the numerical data (i.e., by use of a semilog plot). No attempt was made to account for a field or temperature-dependent prefactor. The point of Fig. 10 in Guyer and Miller is to show qualitatively that the field degrades the "barrier." Further, the calculation of Guyer and Miller, as stated by them, was for a *discrete* version of the sine-Gordon chain—a feature which is not without significance when making numerical comparisons.

5. The SEH method and the NT method are similar in form since both methods build up the nonequilibrium distribution function from a product ansatz. In the NT method $\hat{\rho}$ is multiplied by

$$\exp\int\frac{dx}{a}w[\theta(x)]\ ,$$

where $w[\theta(x)]$ may depend upon $\theta(x)$, $\nabla\theta(x),\ldots$. In the SEH method ρ is multiplied by

$$\exp\left[\sum_i w(\theta_i)+\sum_i u(\theta_{i+1}-\theta_i)+\cdots\right]\ , \qquad (57)$$

as in Eqs. (37), (40) , ... As the SEH method has been used by I6 and Guyer and Miller Eq. (57) is truncated after the first term (ansatz 1). Büttiker and Landauer argue that in principle this treatment of Eq. (57) is unsuitable. If the modifcation of the relative motion of pairs of particles, etc. (as a consequence of a steady current) were substantial compared to the relative motion permitted by the equilibrium distribution function, then terms like $u,\ldots$ in Eq. (57) would be retained. We find no evidence that important deviations from the Hartree-like result occur. [The inclusion of terms like u in Eq. (57) leaves unchanged the discrepancy between the low-temperature results of the two methods, i.e., $T^{-1/2}$ vs $T^{-3/2}$.]

6. The NT employing the basic ansatz in the SE, can, in principle, develop a hierarchy of equations for the distribution functions and currents in terms of the normal modes of the critical nucleus. BL proceed by setting *all* except one of the components of the N-particle current to zero (pointwise). This restriction

reduces the basic ansatz to

$$P[\theta(x)] = e^{W(\eta_0)} P_0[\bar{\theta}(x), \eta_0\eta_1\cdots] \ . \tag{58}$$

7. The above ansatz, Eq. (58), appears as a reasonable description of the behavior of the system near the critical nucleus. However, its utility away from the critical nucleus is unclear. BL proceeds as follows: near the critical nucleus the probability distribution function is taken to be

$$\left[\theta(x) = \bar{\theta}(x) + \sum_\nu \eta_\nu \delta\psi_\nu(x)\right] \ ,$$

$$P[\theta(x)] = P(\bar{\theta}(x); \eta_0\eta_1\cdots)$$
$$= e^{W(\eta_0)} \exp\left[-\beta\left[E(\bar{\theta}(x)) + \tfrac{1}{2}\sum_\nu A_\nu \eta_\nu^2\right]\right] \ .$$

Near the stable chain configuration the probability distribution function is taken to be

$$\left[\theta(x) = \bar{\theta}_s + \sum_\mu \chi_\mu \delta\phi_\mu(x)\right] \ ,$$

$$P[\theta(x)] = P(\bar{\theta}_s; \chi_0\chi_1\cdots)$$
$$= e^{W(\bar{\theta}_s)} \exp\left[-\beta\left[E(\bar{\theta}_s) + \tfrac{1}{2}\sum_\mu j_\mu \chi_\mu^2\right]\right] \ . \tag{59}$$

The function $W(\eta_0)$ is fixed at $\eta_0 << 0$ by setting it equal to the constant $W(\bar{\theta}_s)$

$$W(\eta_0 << 0) = W(\bar{\theta}_s) \ .$$

[Note also $W(\theta)$ in Eq. (59) is not permitted to fluctuate about $\bar{\theta}_s$.] It is hard to assess the significance of these approximations.

8. The procedure employed by Büttiker and Landauer for finding the "duct" keeps the term FR while ignoring another term of order FR, $W(R)$. Thus the procedure employed by BL is strictly correct only for $F \to 0$. One should appreciate that the very complex numerical self-consistent solution to Eq. (39) employed by I6 and by Guyer and Miller was necessary because of this point. In this regard Fig. 7 of Guyer and Miller is illuminating.

9. The NT method as carried out be Büttiker and Landauer is subject to four restrictions on the values of the physical parameters for which it is valid; (i) $k_B T << V_0$, (ii) $n_0\xi << 1$, $\xi^2 = K/V_0$, (iii) $\beta F >> n_0$, and (iv) $F/V_0 << 0$. This latter restriction, to low fields as per item 8 above, makes the theory invalid for the small amplitude nucleus (SAN) case discussed at length by BL.

The nucleation theory method for calculation of the steady-state nucleation current permits one to examine the dynamics of the nucleation process in a physically appealing and analytically tractable way. The usefulness of this method is not invalidated by our criticism of details of its implementation by BL. In summary our criticism of the NT method is of (1) the difficulty in assessing the range over which the ansatz of Eq. (58) would be expected to give a good solution to the problem and (2) the difficulty associated with embedding this method of solution in a systematic procedure. Thus it would seem that for quantitative purposes the nucleation theory method is at present superseded by the SEH method.

ACKNOWLEDGMENT

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