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The sine-Gordon chain. II. Nonequilibrium statistical mechanics

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A calculation of the current carried on the sine-Gordon chain in an external field with viscous damping is formulated in terms of the solution of a Smolouchowski equation. The Smolouchowski equation is solved by employing its relationship to the BBGKY hierarchy and by using transfer-integral techniques. The method of solution is not specific to the sine-Gordon chain and can be usefully employed in examining other nonlinear systems. The solution of the Smolouchowski equation takes the form of a self-consistent equation for the single-particle distribution function; the solution describes the system for all values of the external field. At low field, the current is proportional to the field and due to thermally activated phase solitons; at high field, the current is proportional to the field and the conductivity many orders of magnitude greater than the low-field conductivity. A region of very nonlinear conduction separates the low-field and high-field regimes. It is possible to determine the effects of various perturbations on the conductivity of the sine-Gordon chain.

I. INTRODUCTION

In a study of the system described by the ϕ^4 equation, Krumhansl and Schrieffer found that the statistical mechanics of the system could be regarded as a superposition of the conventional small-oscillation modes and of modes special to the ϕ^4 system, solitary waves or soliton modes.[1] This finding suggested a generalization that has proved very useful in attempting to understand the statistical mechanics of nonlinear systems; the low-temperature statistical mechanics of systems possessing solitary wave (or soliton) solutions is well approximated by a superposition of the conventional small-oscillation modes and of the soliton modes. Much recent work has given ample evidence of the usefulness of this suggestion in a variety of applications.[2,3]

Among the most interesting nonlinear systems that one might examine is the sine-Gordon chain. The sine-Gordon equation is known to describe many different kinds of physical systems, and the mathematical properties of this equation have been studied extensively. For example the "phase soliton," a possible low-temperature charge-carrying mode of a charge-density wave, is the soliton of the sine-Gordon equation.[4] The sine-Gordon soliton has been studied in the presence of impurities, a sine gradient, an electric field with damping,[5] etc. The equilibrium statistical mechanics of the sine-Gordon chain has been described by Gupta and Sutherland[6] and others.[7,8] From these studies a simple picture of the low-temperature statistical mechanics of the sine-Gordon chain emerges; the equilibrium properties of the chain are described by a gas of noninteracting solitons.[7,8] The identification of the sine-Gordon soliton with a charge-carrying entity in a charge-density wave[4] suggests that the solitons may be seen directly, against the background of conventional modes of motion, in experiments that probe the nonequilibrium properties of the system. For example, the sine-Gordon soliton could be driven by an electric field and make a contribution to the current. The response of the sine-Gordon chain to small external fields provides a direct probe of the existence of the nonlinear excitations (the entities in the system that owe their existence to its nonlinearity, the solitons), whereas the response of the chain to large external fields can modify the nonlinearity and provide a complementary probe of the chain's nonlinear structure. Thus, it is interesting to consider the response of the sine-Gordon chain to both weak and strong external fields; i.e., to examine both the linear and nonlinear response.

The purpose of this paper is to describe the response of the sine-Gordon chain to an external field. We calculate the properties of the chain in the large-damping limit in which the Fokker-Planck equation for the distribution function can be reduced to a Smolouchowski equation. We solve the Smolouchowski equation for the configuration-space distribution function by exploiting the relationship of that equation to the BBGKY hierarchy and employing transfer-integral techniques.[9] We are able to describe the nonlinear evolution of the current in response to an external field, the effect of impurities on the current, etc. The organization of this paper is as follows. In Sec. II we describe a model for the sine-Gordon chain, the nature of the basic modes of the chain, and our qualitative expectation for the response of the chain to an external field. In Sec. III we set out the Smolouchowski equation and describe a general method of solution. We examine three different cases in detail for arbitrary external field and (i) zero coupling, (ii) weak coupling, and (iii) strong coupling. Our final result, valid for any field and any coupling, is in the form of a self-consistent equation for the single-particle distribution function. In Sec. IV, we describe the results of analytic examination of our solution for the Smolouchowski equation. We show that the current is carried by phase solitons at low field and we examine a number of asymptotes against which we can test the numerical work. In Sec. V we display the results of numerical implementation of the solution from Sec. III; (e.g., current versus field, field evolution of the single-particle density, etc.) and we discuss the basic features of the results, their possible application to charge-density waves, etc. In Sec. VI we describe the effect of various kinds of impurities and defects on the conduction properties of the chain. We summarize our results in Sec. VII. Some details that support the argument in the body of the paper are given in Appendixes A and B.

II. DESCRIPTION OF THE SINE-GORDON CHAIN

The system we wish to consider is a chain of torsion-coupled pendula described by

$$H=\sum_{i=1}^{N}\frac{1}{2}I\omega_i^2+\sum_{i=1}^{N}\left[-E_1\cos\theta_i+\tfrac{1}{2}E_2(\theta_{i+1}-\theta_i)^2\right], \quad (1)$$

where θ_i, the angle of pendulum i, is called the phase of pendulum i, E_1 is a measure of the gravitational potential barrier (see Fig. 1), and E_2 is a measure of the strength of the torsion spring that couples pendulum $i+1$ to pendulum i. We may apply a constant external torque to each pendulum by adding

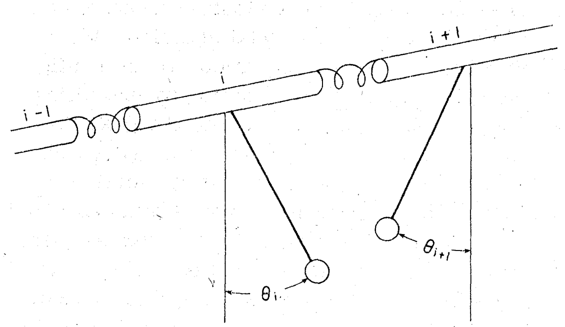

FIG. 1. Sine-Gordon chain. The sine-Gordon chain is modeled by a linear array of pendula. Each pendulum is in the single-particle field due to gravity ($-E_1\cos\theta_i$, $E_1=mgR$) and coupled to its near neighbors by a torsion spring $\frac{1}{2}E_2(\theta_{i+1}-\theta_i)^2$. A constant torque, the external field, is exerted on each pendulum separately by wrapping a string (from which a second mass hangs) around its axle $-E_0\theta_i$.

$$V_e(1\ldots N)=-\sum_{i=1}^{N}E_0\theta_i \quad (2)$$

to Eq. (1). This constant torque tends to drive the phase of each pendulum toward large positive values. We discuss the chain regarding the gravitational torque and torsion-spring torque from Eq. (1) as an internal field and the constant torque from Eq. (2) as an external field.

Among the fundamental modes of the sine-Gordon chain, with the external field set to zero, are the phonon modes associated with small oscillations of the pendula from their equilibrium positions ($\theta_i=0$). For these modes the dispersion relation is

$$\omega_\nu^2=\omega_1^2+\omega_2^2\sin^2\pi\nu\,, \quad (3)$$

where $\nu=n/2N$, $\omega_1^2=E_1/I$, and $\omega_2^2=4E_2/I$. There is also a system of small-oscillation modes for $|\theta_i-\pi|\ll\frac{1}{2}\pi$. In addition to the small-oscillation modes of the chain there are kink or soliton modes.[10] These modes correspond to the optimum way in which the chain can have a kink, a change in the phase from $2\pi m$ to $2\pi(m\pm1)$. Of course, the chain would prefer not to have a kink but if it must have a kink there is a best way to do it (see Fig. 2). The two basic potential energies in Eq. (1) compete to determine the kink energy and size—the barrier energy $-E_1\cos\theta_i$ is minimized by getting the kink over the barrier as soon as possible and having the least number of pendula on the barrier—the elastic energy or energy due to phase gradient $\frac{1}{2}E_2(\theta_{i+1}-\theta_i)^2$ attempts to stretch out any change in phase that must occur. Thus, for a kink of length l the potential energy is approximately

$$l[E_1+E_2(2\pi)^2/l^2]=E_{\rm pot}(l)\,. \quad (4)$$

This energy is a minimum for $l\simeq(E_2/E_1)^{1/2}$ and is of order $(E_2E_1)^{1/2}$. A careful theory of the sine-Gordon chain in the continuum limit finds that kinks on it are described by solitons[10] with

$$\theta=4\tan^{-1}\exp(x-vt)/d\,, \quad (5)$$

where $d=(E_2/E_1)^{1/2}$ is a measure of the length of the kink. The kinks (solitons) have energy

$$E_\phi=8(E_2E_1)^{1/2}\,. \quad (6)$$

The dynamics of the fundamental modes of motion of the particles on the sine-Gordon chain have been carefully studied. For example, $1,2,\ldots,n$ soliton solutions can be constructed.[11] These solutions permit one to study soliton-soliton collisions, etc. Two kinks with the same sense of phase evolution $2\pi m\to2\pi(m+1)$ are repelled from one another (the kink-kink interaction is repulsive); the kink-antikink interaction is attractive[12] and a

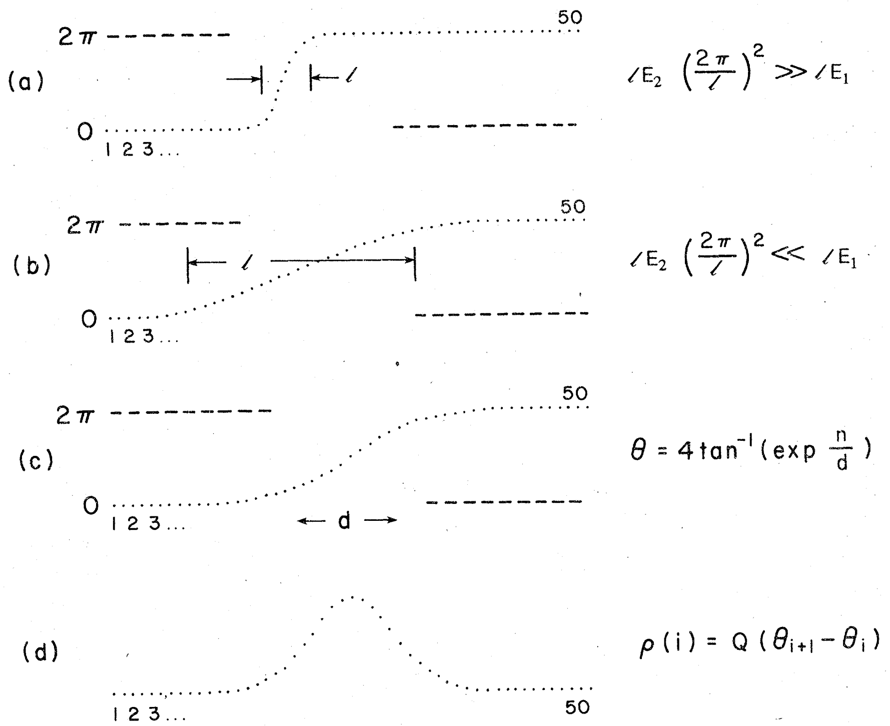

FIG. 2. Optimum kink. The kink size arises from a compromise between the energy to be on the barrier $-E_1 \cos\theta_i$ and the energy of phase gradient. The phase of a particle (angle at which a pendulum lies) is shown as a function of its position along the chain. In (a) the size of the kink l is such that a small number of particles are on the barrier (have phase of order π) at the expense of phase-gradient energy. In (b) the phase gradient has been reduced at the expense of putting many particles on the barrier. In (c) the sine-Gordon soliton is shown; $d = (E_2/E_1)^{1/2}$ is taken as a measure of the size of a kink. The charge density associated with the phase gradient in a kink is shown in (d). A kink and antikink have charge density of opposite sign.

kink-antikink pair will pass through one another or annihilate depending on the details of the energy-transfer process during collision (see Fig. 3). The phonon modes and kink modes on the chain are essentially independent; the phonons suffer only a phase shift upon passing through a kink.[13] In the vicinity of an impurity, a kink distorts in reaction to the local perturbation presented by the impurity and then goes on, having suffered only a phase shift.[5] In the presence of a constant weak external field and damping, the kink is driven by the field against the viscous force and acquires a particlelike terminal velocity. The important result of the many studies of kink dynamics is that the kinks maintain their integrity as fundamental modes of the system under a wide variety of circumstances. We should expect to see the kinks in the equilibrium and nonequilibrium statistical mechanics of the sine-Gordon chain quite possibly behaving as independent particles on the chain.

The equilibrium statistical mechanics of the sine-Gordon chain can be done in the canonical ensemble with

$$F(T,\Phi) = -k_B T \ln Z(T,\Phi)\,, \tag{7}$$

where T is the temperature and Φ is the phase evolution on the chain,

$$\Phi = \int_0^L \frac{\partial\theta}{\partial x}dx = \sum_{i=1}^{N} (\theta_{i+1} - \theta_i) = \theta_N - \theta_0\,. \tag{8}$$

The phase Φ is maintained by a torque

$$\tau = -\frac{\partial F}{\partial \Phi} \tag{9}$$

that does the job of creating the phase on the chain and of holding the phase on the chain.[8] At low temperatures, a phase Φ will go on the chain locally as $\Phi/2\pi$ kinks (this is accomplished by holding pendulum 1 at phase 0 and twisting pendulum N through $\Phi/2\pi$ complete turns. Due to thermal motion these kinks collide with the end of the chain and the torque τ must maintain the phase against the attempt of kinks approaching the end of the chain to change it. At $T = 0$ °K phase $\Phi = 2\pi n$ exists on the chain as an n-kink lattice and is described by the n-soliton solution of the sine-Gordon equation.[6] As the temperature is raised to 0^+ °K, the kink lattice melts and the kinks move freely along the chain approximately like a gas of independent noninteracting particles. Raising the temperature also populates the chain with thermally excited kinks that are created pairwise. The number of thermally excited kinks on the chain is proportional to $\exp(-\beta E_\Phi)$ from Eq. (6).

Suppose that we identify a charge density with the phase gradient[14] of the sine-Gordon chain

$$\rho(x) = Q\frac{\partial\theta(x)}{\partial x}\,, \tag{10}$$

and put this charge density in a uniform electric

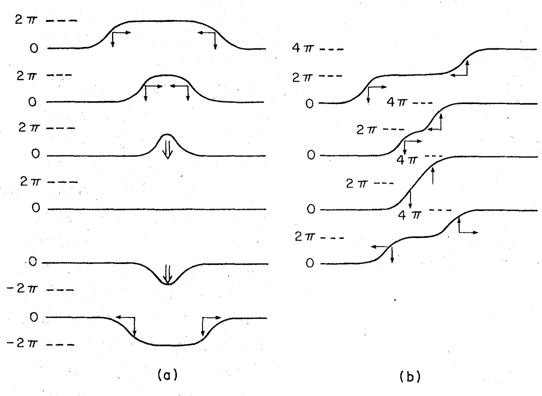

FIG. 3. Kink collisions. The phase as a function of position along the chain is shown in (a) for a segment of chain on which a kink (phase evolution from 0 to 2π) and antikink (phase evolution from 2π to 0) approach one another, collide, and pass through one another. The kink and antikink have equal and opposite charge and are driven toward opposite ends of the chain by the external field. In (b) a segment of chain with two kinks is shown. Two kinks (or antikinks) collide repulsively (they try to twist the intermediate pendula in opposite directions) and come apart carrying their angular momentum in the opposite direction. Kink collisions are more complex than these examples in cases where energy and angular momentum can be converted to other modes of motion on the chain.

field F_0 along the length of the chain

$$H' = \int_0^L F_0 x\rho(x)\,dx \,. \tag{11}$$

The total charge in the system is

$$Q_{\text{total}} = \int_0^L \rho(x)\,dx = Q[\theta(L) - \theta(0)] = Q\Phi \,, \tag{12}$$

where Φ is the phase evolution along the chain. The system is electrically neutral if $\Phi = 0$, i.e., if the chain is periodic over L,

$$\theta(L) = \theta(0) \,. \tag{13}$$

If we integrate Eq. (11) by parts and assume the chain to be periodic, we have

$$H' = -QF_0 \int_0^L \theta(x)\,dx \,. \tag{14}$$

It is this form of H', discretized, that we have used in Eq. (2),

$$H' = QF_0 \int_0^L \theta(x)\,dx = -QF_0 \sum_{i=1}^{N} \theta_i \,, \tag{15}$$

where $E_0 = QF_0$. The discretized form of Eq. (11) is

$$H' = QF_0 \sum_{i=1}^{N} i(\theta_{i+1} - \theta_i) \,. \tag{16}$$

What do we expect to happen to the sine-Gordon chain due to the interaction in Eqs. (11) or (14)? From Eqs. (10) and (11) we see that the charge is identified with phase gradient and that the electric field will drive the phase gradient. Kinks represent the best way for the chain to produce substantial phase change with attendant phase gradient. The kinks contain positive charge and are driven by the electric field; they maintain their integrity in the presence of the electric field and behave like particles. The charge on a kink is

$$Q_K \equiv Q \int_0^L dx \frac{\partial}{\partial x} \tan^{-1} e^{x/\xi} = Q\pi \,, \tag{17}$$

and the kink is driven toward $x = L$ by the field; the charge on an antikink is $-Q_K$ and the antikink is driven toward $x = 0$ by the field.

For the purpose of developing a physical picture of the behavior of the sine-Gordon chain, we may consider it analogous to a washboard[15] (the periodic washboard surface in combination with Earth's gravitational field represents the $-E_1 \cos\theta$ part of the potential energy) on which we have placed a string of beads that are coupled to one another by weak springs [the springs represent the $\frac{1}{2}E_2(\theta_{i+1} - \theta_i)^2$ part of the potential energy]. The effect of the external field is simulated by tipping the washboard up at an angle. (See Fig. 4.) When the field is zero the beads lie at a particular average phase, for example, $2\pi m$ as in Fig. 4; kinks are present on the chain in numbers proportional to $e^{-\beta E_\Phi}$. If we fix the ends of the chain (nail down the end at $x = 0$ and the end at $x = L$) and tip the washboard up at an angle, the phase will evolve so as to reduce the energy of the chain by pushing positive phase gradient to large x and negative phase gradient to small x. The phase will evolve as kinks and the chain configuration shown in Fig. 4 results. As the washboard is tipped to large angles the barrier height is degraded so that the barrier-energy–elastic-energy compromise that gives rise to kinks becomes less and less important to phase evolution. In the limit of large external field, the washboard tipped up on end, the chain of beads hangs as a catenary and there are no vestiges of the kinks.

The situation above, chain, washboard, and fixed end points, is studied in equilibrium statistical mechanics, since, following an initial response as the external field is turned on (after the washboard is tipped) the system resides in equilibrium; there are no currents or fluxes in the system. Consider the situation in which the two ends of the chain are fixed relative to one another $\theta(L) = \theta(0)$ but are *otherwise free to move*. Then when the washboard is tipped up on end the chain of beads slides down it in response to the field.

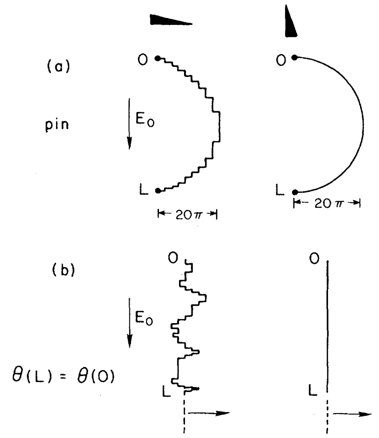

FIG. 4. The washboard model. A qualitative picture of the sine-Gordon chain in an external field is provided by the model of an elastic chain on a washboard. When the ends of the chain are pinned and the field is weak, (a) the phase evolves to take advantage of the energy lowering in the field. Positive phase gradient (in the form of kinks) moves toward L and negative phase gradient (in the form of antikinks) moves toward 0. In low-field phase evolution (and phase gradient) occurs locally as kinks. In high field, the barrier that leads to kink formation is completely overridden by the field, phase evolution occurs nonlocally on the chain; the chain hangs in a catenary. (b) When the ends of the chain are free to move [e.g., $\theta(L)=\theta(0)$] the chain is driven down the washboard by the field. The uniform average motion of the chain is accomplished in low field by kink pair creation followed by the motion of the + and − charged parts of the kink pair in opposite directions. At high field, the chain is driven down the washboard as a rigid object.

The chain will eventually reach a steady state in which it advances down the washboard at a constant rate. Phase gradient resides on the chain in kinks and the chain moves down the washboard by pushing kinks and antikinks in opposite directions (see Fig. 4). There is a continual evolution of the average phase of the chain,

$$\sum_{i=1}^{N} \dot{\theta}_i \neq 0 ,$$

brought about by the continual flow of kinks toward $x=L$ and antikinks toward $x=0$. (The periodic boundary condition means that a kink leaving the chain at $x=L$ returns at $x=0$ as a kink.) If we define a current appropriate to the charge in Eq. (10), we have

$$j(x) = -Q\frac{\partial\theta(x)}{\partial t} \tag{18}$$

or

$$j = Q\langle\dot{\theta}_i\rangle . \tag{19}$$

This current flows on the chain and $\langle\dot{\theta}_i\rangle$ is the same for all i by continuity. Thus, in the presence of an external field *and* with periodic boundary conditions the chain is a nonequilibrium system.

To study certain of the nonequilibrium properties of the sine-Gordon chain we employ the Smolouchowski equation. This equation has been derived for the sine-Gordon chain from the Fokker-Planck equation by Trullinger.[16] The Smolouchowski equation follows from (i) taking the equation of motion of a particular pendulum to be

$$I\dot{\omega}_i = -E_1 \sin\theta_i + E_2(\theta_{i+1} + \theta_{i-1} - 2\theta_i) + E_0 - \eta I\omega_i + F_i(t) , \tag{20}$$

where η is a phenomenological viscosity and $F_i(t)$ is a thermal noise source with properties

$$\langle F_i(t)F_j(t)\rangle = 2\, Ik_B T\eta\delta_{ij}\delta(t) , \tag{21}$$

and (ii) assuming the viscous damping of the motions of the particles is sufficiently strong that, on the relevant time scale, the particles are in velocity equilibrium with the Maxwell-Boltzmann distribution function,

$$\exp(-\tfrac{1}{2}\beta I\omega_i^2) .$$

Under these conditions, the nonequilibrium distribution function we require is the configuration-space distribution function $\sigma(1\cdots N)$ which obeys the Smolouchowski equation

$$\frac{\partial\sigma(1\cdots N)}{\partial t} = \frac{k_B T}{I\eta}\sum_{i=1}^{N}\frac{\partial}{\partial i}\left(\exp[-\beta U(1\cdots N)] \times\frac{\partial}{\partial i}\{\exp[\beta U(1\cdots N)] \times\sigma(1\cdots N)\}\right) \tag{22}$$

It is this Smolouchowski equation (SE) for the sine-Gordon chain that we study in this paper.

In this section we have described a system of torsion-coupled pendula in an external field. This system is described by the sine-Gordon equation; it is a mechanical analog for models of a variety of physical systems that are of considerable interest, e.g., dislocations, epitaxial crystal growth, proximity-coupled Josephson junctions, the Josephson transmission line, charge-density waves, etc.

III. SOLUTION TO THE SMOLOUCHOWSKI EQUATION AND THE CURRENT

The Smolouchowski equation (SE) describes the motion of the N-particle-configuration distribution function through configuration space under the condition of heavy damping; it is an equation for the diffusion of the configuration-space distribution function through configuration space:

$$\frac{\partial\sigma(1\cdots N)}{\partial t}=\frac{k_BT}{I\eta}\sum_{i=1}^{N}\frac{\partial}{\partial i}\left(\exp[-\beta U(1\cdots N)]\times\frac{\partial}{\partial i}\{\exp[\beta U(1\cdots N)]\times\sigma(1\cdots N)\}\right). \quad (23)$$

The potential energy $U(1\cdots N)$ in Eq. (23) is the sum of the internal potential energy that determines the equilibrium behavior of the system, Eq. (1),

$$V(1\cdots N)=-E_1\sum_{i=1}^{N}\cos\theta_i+\frac{E_2}{2}\sum_{i=1}^{N}(\theta_{i+1}-\theta_i)^2\,, \quad (24)$$

and the external potential energy that drives the system away from equilibrium, Eq. (2),

$$V_e(1\cdots N)=\sum_{i=1}^{N}V_e(i)=-\sum_{i=1}^{N}E_0\theta_i\,. \quad (25)$$

Equation (23) may be viewed in the form of a continuity equation

$$\frac{\partial\sigma(1\cdots N)}{\partial t}+\vec{\nabla}_N\cdot\vec{J}(1\cdots N)=0\,, \quad (26)$$

where $\sigma(1\cdots N)$ is the probability density and $\vec{J}(1\cdots N)$ is the corresponding probability current (here ∇_N is the N-particle gradient). Integration of Eq. (26) over $dn+1\cdots dN$ yields a sequence of conservation laws for the probability densities $\sigma(1\cdots n)$,

$$\frac{\partial\sigma(1\cdots n)}{\partial t}+\vec{\nabla}_n\cdot\vec{J}(1\cdots n)=0\,. \quad (27)$$

The single-particle probability density obeys

$$\frac{\partial\sigma(1)}{\partial t}+\vec{\nabla}_1\cdot\vec{J}(1)=0\,, \quad (28)$$

where

$$J(1)=\frac{1}{\tau}\int d2\cdots dN\left(\frac{\partial\sigma(1\cdots N)}{\partial 1}+\sigma(1\cdots N)\times\frac{\partial\beta U(1\cdots N)}{\partial 1}\right), \quad (29)$$

and $\tau\equiv k_BT/(I\eta)$. In steady state $\partial\sigma(1)/\partial t=0$ and the current $J(1)$, the probability current for particle 1 (see Fig. 5), is a constant $J(1)=\overline{W}$. Thus we take the average rate of motion of θ_1 to be given by

$$\langle\dot{\theta}_1\rangle=2\pi\overline{W}\,, \quad (30)$$

where 2π is the phase evolution and the steady-state current $\overline{W}$ is a measure of the rate of this phase evolution. The quantity $\langle\dot{\theta}_1\rangle$ is related to j, the current carried by the system (see Sec. II). We have

$$j=Q\langle\dot{\theta}_i\rangle=2\pi Q\overline{W}\,. \quad (31)$$

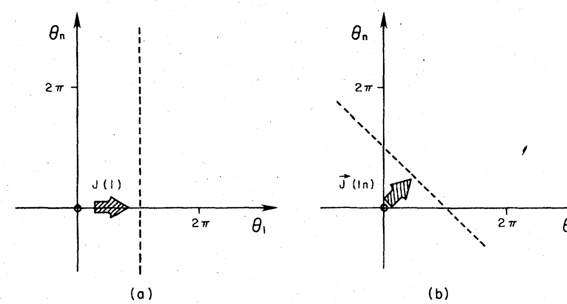

FIG. 5. Calculation of the current. The steady-state solution to the Smolouchowski equation with a nonzero external field involves the determination of the steady probability currents in configuration space, e.g., $J(1)$, $J(1n)$. The steady current $J(1)$ is a measure of the rate of evolution of pendulum 1 from θ_1 to the left of the partition to θ_1 to the right of the partition. This probability current is related to $\langle\dot{\theta}_1\rangle$ and the current. An analogous discussion may be given by the joint probability currents $J(1n)$, $J(1nm)$, ...

The relatively simple form of Eq. (31), relating j to the steady-probability current $\overline{W}$ in configuration space, results from the relationship of the current to the average rate of phase evolution and, in turn, from the relationship of the average rate of phase evolution to the probability current in configuration space $[j\propto\dot{\theta}\propto J(1)]$. No equivalently simple results are available for the energy current or other defined fluxes.

It is possible to define a variety of joint-probability densities and joint currents, e.g., $\sigma(1n)$ and $\vec{J}(1n)$, and to discuss the current across a partition in configuration space like that shown in Fig. 5. In general, we seem to find that the behavior of the joint currents are plausibly related to the behavior of the joint-probability densities. For example, when 1 and n are close to one another (close as measured by the probability that a kink lies between 1 and n) their phase evolution is coordinated and when 1 and n are far apart their phases evolve independently.[1]

From Eq. (31) we see that the current is given by $\overline{W}$, the steady-probability current. It is the current we are interested in calculating. Thus, in dealing with the SE we focus our attention relatively narrowly on the determination of $\overline{W}$. As a first step in the solution to the SE we employ the relationship between the equations of motion for the n-particle nonequilibrium distribution functions and the equations of motion for the n-particle equilibrium distribution functions. The latter equations are the well-known BBGKY equations.

A. The BBGKY hierarchy

For a system of N particles in equilibrium with a system of "internal" forces we have the N-

particle density given by

$$\rho(1\cdots N)=\prod_{i=1}^{N}\phi(i)^2\prod_{i<j}f(ij)^2\,, \qquad (32)$$

where $\phi(i)^2=e^{-\beta V(i)}$, $V(i)$ is the single-particle potential for particle i, and $f(ij)^2=e^{-\beta V(ij)}$, $V(ij)$ is the pair potential between particles i and j. The n-particle densities are defined by

$$\rho(1\cdots n)=\int d(n+1)\cdots dN\,\rho(1\cdots N)\,. \qquad (33)$$

The BBGKY equations follow from taking ∇_1 on the left and right of Eq. (33). The result is

$$\vec{\nabla}_1\rho(1\cdots n)=\rho(1\cdots n)\vec{\nabla}_1[\ln\phi(1)^2]+\rho(1\cdots n)\times\vec{\nabla}_1\sum_{j=2}^{n}\ln f(1j)^2+\sum_{j=n+1}^{N}\int dj\,\rho(1\cdots n+1)\times\vec{\nabla}_1\ln f(1j)^2\,. \qquad (34)$$

The first few BBGKY equations are

$$\frac{\partial}{\partial 1}\rho(1)+\rho(1)\frac{\partial}{\partial 1}\beta V(1)+\sum_{j=2}^{N}\int dj\,\rho(1j)\frac{\partial}{\partial 1}\beta V(1j)=0\,,$$

$$\frac{\partial}{\partial 1}\rho(12)+\rho(12)\frac{\partial}{\partial 1}\beta V(1)+\rho(12)\frac{\partial}{\partial 1}\beta V(12)+\sum_{j=3}^{N}\int dj\,\rho(12j)\frac{\partial}{\partial 1}\beta V(1j)=0$$

$$\cdots\,. \qquad (35)$$

The SE for the n-particle distribution functions $\sigma(1\cdots n)$ can be written in a form similar to the corresponding BBGKY equations. If we integrate Eq. (23) over $2\cdots N$, $3\cdots N$, etc., we obtain

$$\frac{\partial\sigma(1)}{\partial 1}+\sigma(1)\frac{\partial\beta V(1)}{\partial 1}+\sum_{j=2}^{N}\int dj\,\sigma(1j)\frac{\partial\beta V(1j)}{\partial 1}+\sigma(1)\frac{\partial\beta V_e(1)}{\partial 1}=\overline{W}\tau\,, \qquad (36)$$

$$\frac{\partial}{\partial 1}\left(\frac{\partial\sigma(12)}{\partial 1}+\sigma(12)\frac{\partial\beta V(1)}{\partial 1}+\sigma(12)\frac{\partial}{\partial 1}\beta V(12)+\sum_{j=3}^{N}\int dj\,\sigma(12j)\frac{\partial\beta V(1j)}{\partial 1}+\sigma(12)\frac{\partial\beta V_e(1)}{\partial 1}\right)+\frac{\partial}{\partial 2}(\text{same for 1 and 2 interchanged})=0$$

$$\cdots\,. \qquad (37)$$

In writing Eq. (36) we have used the first integral of Eq. (29) in terms of the steady probability current $\overline{W}$. The single-particle potential $V_e(i)$ in Eqs. (36) and (37) is that of the external field that drives the system away from equilibrium. If we put $V_e(i)=0$ Eqs. (36), (37), ... are solved by

$$\sigma(1)=\rho(1)\,, \qquad (38a)$$

$$\sigma(12)=\rho(12)\,, \qquad (38b)$$

$$\sigma(123)=\rho(123)\,, \qquad (38c)$$

$$\cdots\,.$$

This suggests that we seek the solution to Eqs. (36), (37), ... in the form

$$\sigma(1)=\rho(1)e(1)\,, \qquad (39a)$$

$$\sigma(12)=\rho(12)e(12)\,, \qquad (39b)$$

$$\cdots$$

$$\sigma(1\cdots N)=\rho(1\cdots N)e(1\cdots N)\,. \qquad (39')$$

In proceeding this way we assume we know or can learn $\rho(1)$, $\rho(12)$, ..., by solution of the equilibrium problem and that $e(1)$, $e(12)$, ..., are to be found.[17] Equations (36), (37), ..., become a system of coupled equations for $e(1)$, $e(12)$, ... These are

$$\rho(1)\frac{\partial e(1)}{\partial t}=\frac{1}{\tau}\frac{\partial}{\partial 1}\left[\rho(1)\left(\frac{\partial e(1)}{\partial 1}+e(1)\frac{\partial\beta V_e(1)}{\partial 1}+\sum_{j\neq 1}^{N}\int dj\,\frac{\rho(1j)}{\rho(1)}[e(1j)-e(1)]\frac{\partial\beta V(1j)}{\partial 1}\right)\right]\,, \qquad (40a)$$

$$\rho(12)\frac{\partial e(12)}{\partial t}=\frac{1}{\tau}\frac{\partial}{\partial 1}\left[\rho(12)\left(\frac{\partial e(12)}{\partial 1}+e(12)\frac{\partial\beta V_e(1)}{\partial 1}+\sum_{j=3}^{N}\int dj\,\frac{\rho(12j)}{\rho(12)}[e(12j)-e(12)]\frac{\partial\beta V(1j)}{\partial 1}\right)\right]+(\text{1 and 2 interchanged})\,, \qquad (40b)$$

$$\cdots$$

$$\rho(1\cdots N)\frac{\partial e(1\cdots N)}{\partial t}=\frac{1}{\tau}\sum_{i=1}^{N}\frac{\partial}{\partial i}\left[\rho(1\cdots N)\left(\frac{\partial e(1\cdots N)}{\partial i}+e(1\cdots n)\frac{\partial\beta V_e(i)}{\partial i}\right)\right]\,. \qquad (40')$$

In the steady state Eq. (40a) reduces to

$$\bar{W}\tau = \rho(1)\left(\frac{\partial e(1)}{\partial 1} + e(1)\frac{\partial \beta V_e(1)}{\partial 1} + e(1)\beta\tilde{F}(1)\right) , \quad (40a')$$

where $\tilde{F}(1)$ is an effective single-particle field. Each of these equations, whether time dependent or not, couples the various nonequilibrium factors $e(1)$, $e(12), \ldots$, to one another; with the exception of Eq. (40′) for $e(1 \cdots N)$. By virtue of being unreduced, the N-particle distribution function couples only to itself. We are able to solve Eqs. (40) in several cases. The special cases are delineated by values of the basic parameters that characterize the system. These are: $\lambda_1 = \beta E_1$, the ratio of the barrier height to the temperature; $\lambda_2 = \beta E_2$, the ratio of the torsion coupling to the temperature; $\lambda_0 = \beta E_0$, the ratio of the external field (applied torque) to the temperature; $d = (\lambda_2/\lambda_1)^{1/2} = (E_2/E_1)^{1/2}$, d = measure of the length of a kink (soliton); $\beta E_\phi = 8(\lambda_1\lambda_2)^{1/2}$, the ratio of the energy to create a kink (soliton) to the temperature; $q = 4\lambda_1\lambda_2$, the parameter of the Mathieu-equation approximation to the transfer integral, TI, problem.[8]

B. Case 1

The zero-coupling limit is referred to as the Ambegaokar-Halperin (AH) limit; the basic equations were solved by AH in their study of thermal noise in a Josephson junction.[18] In this limit all particles behave independently and the n-particle distribution function is the product of n equivalent single-particle distribution functions. Equations (40) reduce to

$$\frac{\bar{W}\tau}{\rho(1)} = \frac{\partial e(1)}{\partial 1} + \lambda_0 e(1) . \quad (41)$$

This equation is to be solved for $e(1)$ subject to the constraints

$$\int_0^{2\pi} d\theta\, \sigma(\theta) = 1 \quad (42)$$

and

$$\sigma(\theta + 2\pi m) = \sigma(\theta) . \quad (43)$$

Equation (42) follows from our choice of normalization of the single-particle distribution function. The periodicity in $\sigma(\theta)$ [we also have $\sigma(\theta_1 + 2\pi m, \theta_2 + 2\pi m, \ldots, \theta_n + 2\pi m) = \sigma(1 \cdots n)$] follows from the observation that in steady state one cannot make an observation that will determine the absolute phase on the chain. The periodicity of $\sigma(\theta)$ implies periodicity for $e(\theta_1)e(\theta_1\theta_2), \ldots$, since $\rho(\theta_1), \rho(\theta_1\theta_2), \ldots$, are periodic. We solve Eq. (41) by writing

$$e(\theta) = e^{w(\theta)} , \quad (44)$$

with $w(\theta + 2\pi m) = w(\theta)$. We have

$$\frac{\partial w(\theta)}{\partial \theta} = -\lambda_0 + \frac{\bar{W}\tau}{\rho(\theta)e(\theta)} . \quad (45)$$

Thus,

$$w(\theta) - w(0) = -\lambda_0\theta + \bar{W}\tau \int_0^\theta \frac{d\theta}{\rho(\theta)e(\theta)} , \quad (46)$$

so that putting θ equal to 2π yields

$$\bar{W}\tau = \frac{2\pi\lambda_0}{\int_0^{2\pi} d\theta/\sigma(\theta)} . \quad (47)$$

If we return Eq. (47) to Eq. (46) we have an implicit equation for $w(\theta)$,

$$w(\theta) = \lambda_0 \frac{-\theta + 2\pi \int_0^\theta d\theta/\sigma(\theta)}{\int_0^{2\pi} d\theta/\sigma(\theta)} , \quad (48)$$

since $\sigma(\theta) = \rho(\theta)\, e^{w(\theta)}$ and $\rho(\theta)$ is known. In Eq. (48) we have put $w(0) = 0$ since $e^{w(0)}$ is a constant that can be absorbed in the normalization of $\sigma(\theta)$, Eq. (42). The set of equations that constitutes a solution to Eq. (41) subject to the constraints of Eqs. (42) and (43) is Eqs. (47) and (48).

(a) Equation (48) is an implicit equation for $w(\theta)$ [$\sigma(\theta) = \rho(\theta)e^{w(\theta)}$]. In the AH limit an explicit but cumbersome equation can be derived for $w(\theta)$.[18] The implicit form in Eq. (48) is quite simple and has much greater usefulness.

(b) Equation (47) gives the current in terms of an integral over the inverse of $\sigma(\theta)$. Two important points emerge: (1) the current is related to an average property of the nonequilibrium distribution function of a single particle, and (ii) the current is sensitive to the nonequilibrium distribution function where it is small, i.e., in that region of configuration space where $\sigma(\theta)$ is most difficult to learn. Below, we will discuss the solution of Eq. (23) for the current in several approximations that are fancier than this one. Nonetheless, the essential features of the solution, as embodied in Eqs. (47) and (48) and remarked on here, remain.

C. Case 2

The weak-coupling limit corresponds to the case in which the size of a kink is of the order of only a few units, i.e., $d = (E_2/E_1)^{1/2} \lesssim 1$. The idea of this limit is that the coupling is present so that we must go beyond the AH solution but at the same time it is sufficiently weak that correlations of only a few units need be considered. To solve Eqs. (40) we make the ansatz

$$\sigma(\theta) = \rho(\theta)e(\theta) ,$$
$$\sigma(\theta_i\theta_j) = \rho(\theta_i\theta_j)e(\theta_i)e(\theta_j) . \quad (49)$$

Then Eq. (40a′) closes without recourse to the higher-order equations and a Hartree-like self-consistent equation for $e(1)$ emerges. The detailed set of equations, employed in carrying through the consequences of the ansatz in Eq. (49), is described in Appendix A. We employ the numerical implementation of these equations to test reduction to the AH limit and the weak coupling limit of the more general solution described below as case 3.

D. Case 3

In the strong-coupling limit we make no restriction on the strength of the unit-unit coupling or on the strength of the external field. The system of equations that gives $\sigma(1), \sigma(12), \ldots$ is coupled and could be solved at low order by some decoupling scheme, e.g., as case 2 above (however, low-order decoupling only works for $d \lesssim 1$). We go directly to the N-particle equation, Eq. (40′). We make the ansatz

$$e(1 \cdots N) = e(1)e(2) \cdots e(N)\,, \tag{50}$$

and we write

$$e(i) = e^{w(i)}\,. \tag{51}$$

Equation (40′), the equation for the N-particle nonequilibrium distribution function, becomes

$$\tau\rho(1\cdots N)\frac{\partial}{\partial t}\,e(1\cdots N) = \sum_i \frac{\partial}{\partial i}\left[\sigma(1\cdots N)\left(\frac{\partial w(i)}{\partial i}+\lambda_0\right)\right]. \tag{52}$$

We integrate this equation on $2,3,\ldots,N$ to obtain

$$\frac{\overline{W}\tau}{\sigma(1)} = \left(\frac{\partial}{\partial 1}+\lambda_0\right) e(1)\,, \tag{53}$$

where

$$\sigma(1) = \int d2 \cdots dN\, \rho(1\cdots N)e(1)\cdots e(N)\,. \tag{54}$$

This equation is the same as Eq. (45) above except that $\sigma(\theta)$ on the left-hand side of Eq. (31) is found by a more complicated prescription. To be able to use Eq. (53) and its consequences we must be able to learn $\sigma(\theta)$. But from Eqs. (54) and (51) it is straightforward to find $\sigma(\theta)$ using transfer-integral techniques.[6,17] We have

$$\sigma(\theta) = \phi_0(\theta)\psi_0(\theta)\,, \tag{55}$$

where ϕ_0 and ψ_0 are the left- and right-hand ground-state solutions of the transfer-integral equations

$$\int d2\, e^{-\beta V(1)} e^{w(1)} \exp[-\tfrac{1}{2}\lambda_2(\theta_2-\theta_1)^2]\psi_\nu(\theta_2) = e^{-\beta\epsilon_\nu}\psi_\nu(\theta_1)\,, \tag{56a}$$

$$\int d1\, \phi_\nu(1) e^{-\beta V(1)} e^{w(1)} \exp[\tfrac{1}{2}\lambda_2(\theta_2-\theta_1)^2] = e^{-\beta\epsilon_\nu}\phi_\nu(\theta_2)\,. \tag{56b}$$

We remark below on the reduction of these equations to a Schrödinger equation and on a number of practical details associated with the solution to Eqs. (56).[8] The important point that emerges here is that the ansatz of Eqs. (50) reduces the calculation of the N-particle nonequilibrium distribution function to the solution of a pseudoequilibrium problem, with a single-particle potential $V(1) - W(1)$ $[w(1) \equiv \beta W(1)]$, on which transfer-integral techniques can be employed. The complication in this apparently simple result is that $w(\theta)$ is not known but must be obtained self-consistently from Eqs. (48) and (56). With $\sigma(\theta)$ in hand, we proceed as in case 1 above and find

$$\overline{W}\tau = \frac{2\pi\lambda_0}{\int_0^{2\pi} d\theta/\sigma(\theta)}\,, \tag{57}$$

with

$$w(\theta) = \lambda_0 \frac{-\theta + 2\pi\int_0^\theta d\theta/\sigma(\theta)}{\int_0^{2\pi} d\theta/\sigma(\theta)} \tag{58}$$

and

$$\int_0^{2\pi} \sigma(\theta)\, d\theta = 1\,. \tag{59}$$

This is the same set of equations as case 1 except that now $\sigma(\theta)$ is learned self-consistently from Eqs. (48) and (56). The calculations of the current and other properties of the driven sine-Gordon chain are based on this discussion and the equations displayed here [Eqs. (56)–(59)].

It is clear from the development above that a number of other approximations to $\sigma(1\cdots N)$ can be made and carried through to an essentially complete solution for $\sigma(\theta)$, $\overline{W}\tau$, etc.; for example, the ansatz

$$e(1\cdots N) = f(12)f(23)\cdots f(N-1N)\,, \tag{60}$$

or the ansatz

$$e(1\cdots N) = e(1)\cdots e(N)f(12)\cdots f(N-1N)\,. \tag{61}$$

We have looked at the consequence of these approximations and we find no essential features different from those which emerge from Eq. (60). We support this finding with the observation that the current is related to an average property of the single-particle distribution function and that quantity is as well approximated by the ansatz of Eq. (50) as it is by the ansatz of Eq. (60) or the ansatz of Eq. (61). The ansatz of Eq. (50) retains the equilibrium correlations between particles and changes the effective single-particle potential that each particle sees. This appears to be adequate for discussing the current. If one were concerned about the pair correlation function, e.g., $\sigma(12)$ or $\sigma(12)/[\sigma(1)\sigma(2)]$ quite possibly ansatz (60) or ansatz (61) would be more suitable. Finally, we remark that the ansatz of Eq. (50) permits all particles to respond to the external field. If a kink is $d \gg 1$ units long, all of the particles participating in the kink motion and carrying charge are able to respond to the field. This is unlike case 2 which amounted to

$$\sigma(12\cdots N) = e(1)e(2)\rho(1\cdots N),$$

and permitted only local response to the field and failed in numerical studies at $d > 1$.[19]

IV. THE CURRENT

In this section, we describe a number of further details associated with calculating the current from the above prescription. We also display a number of analytic limits and tests in preparation for examining the numerical implementation of Eqs. (57)–(59).

To find the current from Eqs. (57)–(59) we need to find $\psi_0(\theta)$ and $\phi_0(\theta)$ from Eqs. (56) with $w(\theta)$ of Eqs. (56) and (58) self-consistently determined. In solving Eqs. (56) and (58) self-consistently, we have used the differential form of Eq. (56). This is

$$\left(-\frac{1}{2\lambda_2}\frac{d^2}{d\theta^2} - \lambda_1 \cos\theta + w(\theta)\right)\psi_\nu(\theta) = \beta\epsilon_\nu\psi_\nu(\theta). \qquad (62)$$

In paper I we have discussed the limits for which the TI problem can be reduced to a Schrödinger equation. From Eq. (58) we see that $w(\theta) \propto \lambda_0$ so that as $\lambda_0 \to 0$ so does $w(\theta)$ and Eq. (62) reduces to

$$\left(-\frac{1}{2\lambda_2}\frac{d^2}{d\theta^2} - \lambda_1 \cos\theta\right)\psi_\nu(\theta) = \beta\epsilon_\nu\psi_\nu(\theta). \qquad (63)$$

Then $\sigma(\theta) \to \rho(\theta)$, the equilibrium distribution function, and

$$\lim_{\lambda_0 \to 0} \bar{W}\tau = \frac{2\pi\lambda_0}{\int_0^{2\pi} d\theta/\rho(\theta)}. \qquad (64)$$

Thus the low-field current depends upon the behavior of $\rho(\theta)$ where it is small; i.e., in the barrier midway between $2\pi m$ and $2\pi(m+1)$. To learn about $\rho(\theta)$, really $\phi(\theta)$ and $\psi(\theta)$, midway between 0 and 2π, we note that Eq. (63) is the Mathieu equation so that we may take over many of the analytic results available from the study of that equation. To convert Eq. (62) to the Mathieu equation we use $q = 4\lambda_1\lambda_2$ to achieve[20]

$$\left(-\frac{d^2}{d\theta^2} - \frac{q}{2}\cos\right)\psi_\nu(\theta) = 2\beta\epsilon_\nu\lambda_2\psi_\nu(\theta). \qquad (65)$$

This is the Schrödinger equation for a particle in a sinusoidal potential of strength q and its qualitative properties are governed by the parameter q. For $q \to 0$ the particle is almost a plane wave; for $q \gg 1$ the particle is highly localized near $2\pi m$. The parameter q is a special combination of the particle's mass

$$\hbar^2/m \leftrightarrow 1/\lambda_2,$$

and the barrier height that characterizes the single-particle potential

$$V_0 \leftrightarrow \lambda_1,$$

$$mV_0/\hbar^2 \leftrightarrow \lambda_1\lambda_2.$$

In the limit $q \gg 1$ we expect the particle to rarely be in the barrier between $2\pi m$ and $2(m+1)$. We have

$$1/\rho(\pi) = 1/\phi_0(\pi)\psi_0(\pi)$$

and

$$\int_0^{2\pi} \frac{d\theta}{\rho(\theta)} \approx \frac{1}{\rho(\pi)}.$$

Thus in Eq. (64) we find the current proportional to $\rho(\pi)$

$$\bar{W}\tau = 2\pi\rho(\pi)\lambda_0 \propto e^{-\beta E_\phi} \qquad (66)$$

i.e., the current proportional to the number of thermally activated solitons in the system. (See I and Appendix B.) This result is a consequence of the structure of Eq. (57). It is in agreement with our remarks in Sec. II and with the expectation announced by Rice *et al.*[4]

In Appendix B we have tabulated a variety of analytic results on $\sigma(\theta)$, etc., that are useful for examining the solution to Eq. (56), for troubleshooting the numerical work, etc.

Equation (66) for the current in low field can be achieved by any of a variety of treatments of Eq. (57). The principle point of this work is to examine a formulation which can be carried to high field, i.e., $\lambda_0 \to +\infty$, $w(\theta) \neq 0$. In high fields we expect $\sigma(\theta)$ to go to a constant; in the presence of a field that can drive them arbitrarily hard there is no reason for a particle to recognize the barrier. We have $\sigma(\theta) = \text{const}$ and from the norm Eq. (59),

$$\sigma(\theta) = 1/2\pi. \qquad (67)$$

Thus, from Eq. (57) we have

$$\bar{W}\tau = \lambda_0/2\pi. \qquad (68)$$

In this limit ϕ_0 and ψ_0 must approach a constant,

$$\phi_0 \approx \psi_0 \approx 1/\sqrt{2\pi}.$$

This is accomplished in the solution of Eq. (62) by the single-particle potential $w(\theta)$ approaching $-\lambda_1 + \lambda_1\cos\theta$, i.e., exactly canceling the single-particle field given by Eq. (1). As the field is turned from

$\lambda_0 \ll 1$ to $\lambda_0 \gg 1$, the distribution function evolves from one which describes localization near $2\pi m$ to one which is uniform. This evolution is accompanied by an evolution of the self-consistent field $w(\theta)$ from zero to a field that cancels the internal field $-\lambda_1 \cos\theta$.

The current is linear in λ_0 for low field and for high field. The ratio of the low-field current to the high-field current is

$$\frac{\overline{W}(\lambda_0 \to 0)}{\overline{W}(\lambda_0 \to +\infty)} = (2\pi)^2 \rho(\pi)\,, \qquad (69)$$

i.e., the ratio of the low-field to high-field conductivities is proportional to $\rho(\pi)$, $\rho(\pi) \ll 1$. A conductivity change of many orders of magnitude occurs between low and high fields. This nonlinear evolution of the conductivity should occur when E_0 has eroded enough of the barrier, $E_1 \cos\theta$, so as to strikingly reduce the energy required to produce a kink and to permit easy flow of the particles.[21] Thus, it is useful to scale the self-consistent field by λ_1 and to view the potential energy in Eq. (62) as

$$\lambda_1[-\cos\theta + u(\theta)]\,, \qquad (70)$$

where $u(\theta) = \lambda_1^{-1} w(\theta)$.

V. NUMERICAL RESULTS

We have solved the system of self-consistent equations developed in Sec. III to determine the nonequilibrium distribution function, the current, etc., for a variety of values of the basic parameters that characterize the sine-Gordon chain. Details of the results of these calculations are described in this section.

The numerical solution to Eqs. (57)–(59) has been carried out for the values of these parameters noted in Table I. This choice of values of the parameters permits us to examine the behavior of the system as the temperature evolves from low temperature ($\beta E_\phi \gg 1$, $k_B T \ll$ energy to create a kink) to high temperature ($\beta E_\phi \ll 1$) and to watch the evolution of kink conductivity at fixed temperature as the width of the soliton ($d^2 = E_2/E_1$) is varied. In studying Eqs. (57)–(59), we typically fix $q = 4\lambda_1\lambda_2$ and vary λ_1 and λ_2. A study at fixed q for various products $\lambda_1\lambda_2 = \frac{1}{4}q$ is a study of the behavior of the chain at fixed temperature and fixed kink energy as the composition of the size of the kink changes. See rows 1, 2, and 3 of Table I. A study at various q for fixed λ_2/λ_1 corresponds to fixed kink size and energy and varying temperatures. See rows 1, 4, and 5 of Table I.

The length scale for the size of a kink is dimensionless, $d = (\lambda_2/\lambda_1)^{1/2}$ and is approximately the number of pendula or units over which a kink occurs (Fig. 2). The energy scale is not set because the basic parameters are dimensionless—all energies are set relative to $k_B T$. To give the discussion here a definiteness that will help to make it more useful, we arbitrarily choose an energy scale and make the discussion in terms of it. See columns (e) and (f) of Table I.

TABLE I. Basic parameters for numerical work. The values of the basic parameters that describe the system are listed for the five studies described in the text. The energy scale has been set by the choice $T = 1\,°$K for case 1.

Case	(a) q	(b) λ_1	(c) λ_2	(d) d^2	(e) E_ϕ/k_B	(f) T
1	10	0.25	10	40	12.7 K	1.00 K
2	10	1.0	2.5	2.5	12.7 K	1.00 K
3	10	2.5	1.0	0.40	12.7 K	1.00 K
4	7.5	$\frac{1}{8}\sqrt{3}$	$5\sqrt{3}$	40	12.7 K	1.15 K
5	5.0	$\frac{1}{8}\sqrt{2}$	$5\sqrt{2}$	40	12.7 K	1.41 K

A. Behavior of the chain as a function of kink size

The energy required to create a kink is achieved as a result of a compromise between the energy required to have the pendula on the barrier and the elastic energy (i.e., the gradient energy). Studies 1, 2, and 3 of Table I describe chains with kinks of the same energy (it is 12.7 K in our units) but of three different lengths $\sqrt{40}$, $\sqrt{2.5}$, and $\sqrt{0.40}$, respectively. In case 1, the kink is long because the elastic energy is large compared to the barrier energy $E_2 = 10$ K, $E_1 = 0.25$ K. In case 3, the barrier energy is larger than the elastic energy $E_2 = 1.0$ K, $E_1 = 2.5$ K. In this case the kink is less than one unit long and a soliton picture of the kink is approaching the limit of its validity.[22] Certainly if phase 2π can be evolved between neighboring units for less energy than it costs to build a soliton, i.e., if

$$\tfrac{1}{2} E_2 (2\pi)^2 < E_\phi\,,$$

the system will make kinks in this local fashion and solitons (as entities in which the phase evolves smoothly) will not exist. This criterion reduces to $d < 4/\pi^2 \simeq 0.4$. Case 3 approaches this limit.

In Figs. 6–8 we show the results obtained from the solution of Eqs. (57)–(59) for the current. In Fig. 6, we show the evolution of the current as a function of field in the form $\overline{W}\tau$ vs $\lambda_0/\lambda_1 = E_0/E_1$.

(i) At low field $E_0 \ll E_1$, the current is proportional to E_0 and is due to thermally activated kinks (see the discussion in Sec. IV). On Fig. 6, we show a dashed line representing the analytic asymptote for the current. The agreement of the

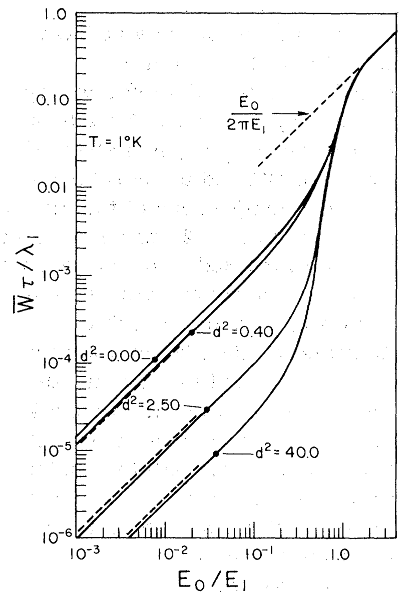

FIG. 6. Current as a function of kink size. The current [in the form $\bar{W}\tau$, Eq. (57)] is plotted as a function of the dimensionless field $\lambda_0/\lambda_1 = E_0/E_1$. These results are from studies 1, 2, and 3 of Table I in which the energy $8(E_1E_2)^{1/2}$ is kept fixed at 12.7 °K, the ambient temperature was 1 °K, and the kink size is varied from $d^2 = 0.40$ to $d^2 = 40$. At low field, the current is proportional to E_0 and due to thermally activated kinks. The nature of these kinks is different according to how the basic energy $(E_1E_2)^{1/2}$ is shared by E_1 and E_2 separately. As $E_1 \to 0$ while E_1E_2 is constant, the kink energy goes asymptotically to the energy of a continuum kink $8(E_1E_2)^{1/2} = E_\Phi$. Away from this asymptote the kink energy is different from E_Φ due to the discrete nature of the chain.

numerical results with the analytic asymptote confirms our picture of the low-field conductivity. We discuss some quantitative aspects of this result later.

(ii) At high field $E_0 \gg E_1$, the current is again proportional to E_0 and is due to the field driving the chain uniformly against the viscous force. Note again that the numerical solution evolves to the analytic asymptote shown by a dashed line.

(iii) Striking nonlinear evolution of the current occurs at $E_0 \approx E_1$ as the field smooths out the barrier.

As λ_1 approaches zero at fixed q, that is as we consider a sequence of chains in which the kink energy is constant but is dominated more and more by the elastic energy, the kink becomes longer and longer, $\lambda_1 \to 0$, and the asymmetry of the completeness relation that is employed in treating the transfer integral disappears.[23] In this limit the transfer integral, current, etc., are characterized by q alone. Thus the evolution of the current that is observed in Fig. 6 at fixed q and λ_0 as we change λ_2/λ_1 is due to the discreteness of the chain. As $\lambda_1 \to 0$ so that $d \gg 1$ the discrete character of the chain is lost and all kinks regardless of their size carry the same current. Universal behavior always obtains in the continuum limit (see I).

The current, as a function of field, changes as the single-particle distribution function changes, Eq. (57). Change in the single-particle distribution function is brought about as it responds to the self-consistent field $u(\theta)$. In Fig. 7, we show the evolution of $\lambda_1[-\cos\theta + u(\theta)]$ as λ_0 evolves from well below the critical field $\lambda_0/\lambda_1 \approx 1$ to above the critical field. As with the current itself, the behavior of $u(\theta)$ at $\lambda_0/\lambda_1 \ll 1$ and $\lambda_0/\lambda_1 \approx 1$ is in reasonable agreement with analytic asymptotes.

In Fig. 8, we show the evolution of the single-particle distribution function $\sigma(\theta)$ as λ_0 evolves. At $\lambda_0/\lambda_1 \ll 1$ the distribution function is pushed mildly away from its equilibrium form as the external field begins to push the pendula up against the barrier. As the external field is increased, the barrier is lowered and $\sigma(\theta)$ evolves towards its high-field form, $\sigma(\theta) = \text{const}$. At high field, the pendula will be found with equal probability at all angles as the field removes all subtlety from the phase-evolution process.

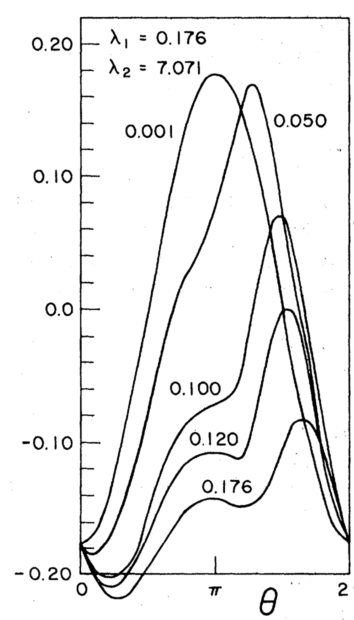

FIG. 7. The effective field. The nonequilibrium single-particle distribution function is determined by the single-particle field $\lambda_1[-\cos\theta + u(\theta)]$, Eq. (70). The single-particle field is shown as the external field varies from $\lambda_0 = 0.001$ to 0.176 (the ratio E_0/E_1 evolves from 0.005 68 to 1.00). As λ_0 varies from 0 to $+\infty$ the single-particle field evolves from $-\lambda_1\cos\theta$ to $-\lambda_1$.

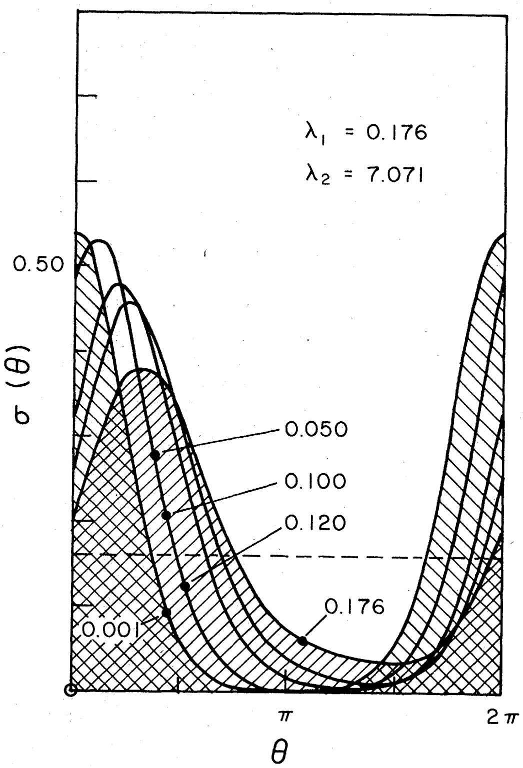

FIG. 8. Single-particle density. The single-particle density given by the self-consistent solution to Eqs. (57)–(59) is shown as a function of angle for five values of the external field, $\lambda_0 = 0.001$, 0.050, 0.100, 0.120, and 0.176. As λ_0 evolves from 0.001 to 0.176 E_0/E_1 evolves from 0.005 68 to 1.00. Compare these results with Fig. 7 which shows the effective single-particle field that generated these densities.

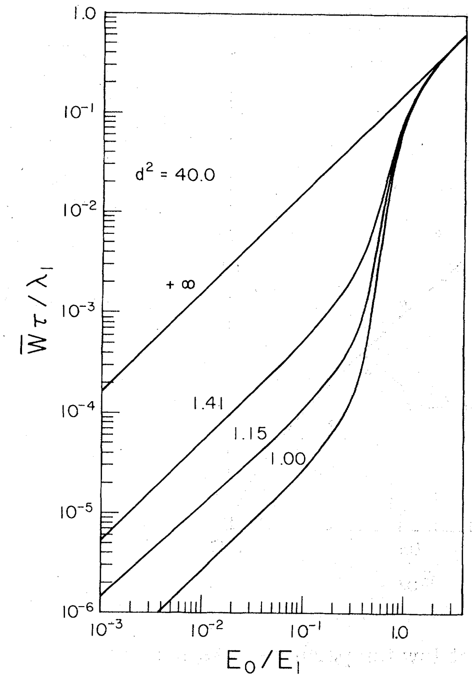

FIG. 9. Current as a function of temperature. The current [in the form $\bar{W}\tau$, Eq. (57)] is plotted as a function of the dimensionless field $\lambda_0/\lambda_1 = E_0/E_1$ for several values of the temperature. These results are from studies 1, 4, and 5 from Table I; the kink size is fixed at $d^2 = 40.0$ and the ambient temperature is 1.00, 1.150, and 1.41 °K. The low-field current is due to thermally activated kinks. From a plot of $\bar{W}\tau$ vs T^{-1} at fixed $E_0 \ll E_1$ we find that the low-field current is carried by kinks with activation energy 10.8 °K. This "empirical" kink energy is close to the analytic asymptote 12.7 °K corresponding to the continuum limit $d^2 \to +\infty$.

B. Behavior of the chain as a function of temperature

In studies 1, 4, and 5 of Table I we have looked at the evolution of the current as a function of field for fixed kink energy and size as the temperature evolves. We show the current as a function of the field for three temperatures in Fig. 9. The qualitative features of the behavior of the current noted above are also seen in Fig. 9. At the lowest fields, the current is carried by thermally activated kinks. We show this in Fig. 10. We have extracted a thermal activation energy by analyzing $\bar{W}\tau$ vs T^{-1} for several values of the field. In Fig. 10(b) we show the activation energy, the slope of $\bar{W}\tau$ vs T^{-1}, as a function of E_0/E_1. On this curve we also show the field dependence of the effective barrier given by the following arguments. The energy to create a kink is $8(E_1 E_2)^{1/2}$. The field tends to degrade the barrier $-E_1 \cos\theta$ that contributes to the kink energy. At field $E_0 \neq 0$, we might take the barrier energy to be

$$b\left(\frac{E_0}{E_1}\right) \equiv \left(\frac{(-E_1\cos\theta - E_0\theta)_{\max} - (-E_1\cos\theta - E_0\theta)_{\min}}{E_1}\right)^{1/2}, \tag{71}$$

see Fig. 10(b). Then the energy to create a soliton is

$$E_\phi(E_0/E_1) = E_\phi b(E_0/E_1)\,. \tag{72}$$

On Fig. 10(a) we have plotted $E_\phi(E_0/E_1)$ from Eq. (72) with E_ϕ chosen to give the result observed in Fig. 9 as $E_0/E_1 \to 0$. We note that $E_\phi(E_0/E_1)$, given by Eq. (72), does a reasonable job of describing the essential features of what we observe in the numerical results. But, certainly, there are clear systematic departures from Eq. (72), e.g., the energy to create a kink is insensitive to the field in first order as $E_0/E_1 \to 0$, unlike Eq. (72).

One of the most striking features of Eq. (57) for the current is the dependence of the current on $\sigma(\theta)$ where it is small. Certainly this is correct

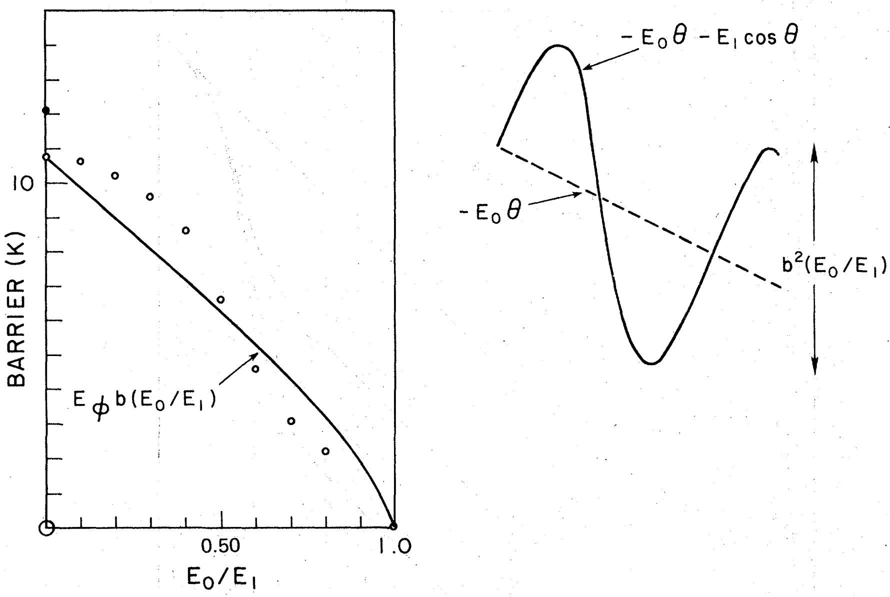

FIG. 10. Barrier height vs external field. The barrier height is plotted as a function of the dimensionless field for $d^2=40$ as open circles. The barrier height is found from an $\overline{W}\tau$ vs T^{-1} analysis of the numerical results shown in Fig. 9. Also shown is a continuous curve given by the simple argument in the text, Eq. (42).

at $\lambda_0 \to 0$ and at low temperature. As evidence of the general validity of this assertion we show in Fig. 11 a plot of $\sigma(\theta)_{\min}$ vs $\overline{W}\tau/\lambda_0$. From Fig. 11 we see that $\overline{W}\tau \propto \sigma(\theta)_{\min}$ behaves qualitatively as

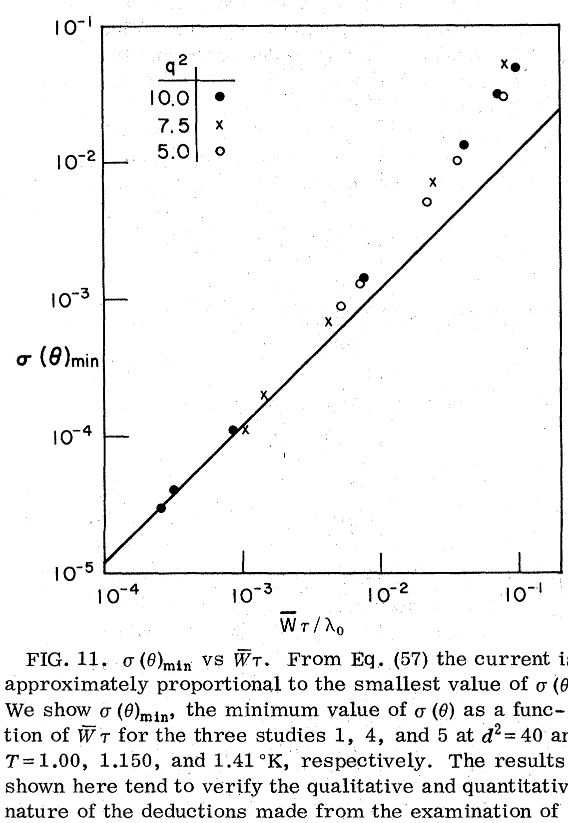

FIG. 11. $\sigma(\theta)_{\min}$ vs $\overline{W}\tau$. From Eq. (57) the current is approximately proportional to the smallest value of $\sigma(\theta)$. We show $\sigma(\theta)_{\min}$, the minimum value of $\sigma(\theta)$ as a function of $\overline{W}\tau$ for the three studies 1, 4, and 5 at $d^2=40$ and $T=1.00$, 1.150, and 1.41 °K, respectively. The results shown here tend to verify the qualitative and quantitative nature of the deductions made from the examination of Eq. (57).

expected, and that the curve has a universal character that suggests that $\sigma(\theta)_{\min}$ is a good indicator of the current.

A basic feature of the behavior of the current on the sine-Gordon chain is that there are two characteristic energies: (a) the energy required to create the thermal equilibrium kinks that are seen in the temperature dependence of the low-field conductivity, and (b) the energy required to degrade the barrier and to permit uniform phase evolution. These energies are E_ϕ and E_1, respectively. We have $E_\phi = 8dE_1 \gg E_1$. This inequality is an essential feature of the kink or soliton picture of local phase evolution.

Certain qualitative features of the dc conductivity measurements of Cohen *et al.*[24] on tetrathiafulvalene-tetracyanoquinodimethane (TTF-TCNQ) at low temperatures are similar to those observed in Figs. 6 and 9. It has been speculated that this conductivity is due to phase solitons, the solitons of the sine-Gordon chain.[9] An essential feature of the data of Cohen *et al.* is that the energy that characterizes thermal excitation at low temperatures is the same as the energy required to degrade the barrier. See Fig. 2 of Cohen *et al.* This empirical fact would seem to be compelling evidence against identification of the conductivity process as a phase-soliton process. Compare our remarks here with the analysis of Wonneberger and Gleisberg.[25]

VI. THE CURRENT IN THE PRESENCE OF PERTURBATIONS

In this section, we briefly discuss the effect that various perturbations on the sine-Gordon chain have on the current. Central to this discussion are two results from above. (i) In the steady state the current is the same for all pendula, $\langle\dot{\theta}_i\rangle=$const for all i, so that if the current is zero for one pendulum it is zero for all pendula. Equivalently, if the current is nonzero for one pendulum it is nonzero for all pendula. (ii) The current, given by Eq. (57), is zero if $\sigma(\theta)$ has a zero for $0\leq\theta\leq 2\pi$. If we limit our discussion of the effects of perturbations to the low-field case we may replace $\sigma(\theta)$ in Eq. (57) by $\rho(\theta)$ (see Sec. IV). Thus the current will vanish if the equilibrium density $\rho(\theta)$ vanishes in the interval $0, 2\pi$.

We consider three perturbations to the chain:

(a) *A pinning site.* This perturbation is a constraint on the location of a pendulum

$$\delta(\theta_i-\Phi) \tag{73}$$

that breaks the translational invariance of the chain. There is no current flow in this case.

(b) *A set of displacement springs.* Along a section of the chain the torsion springs attempt to establish a relative phase between the pendula. This perturbation corresponds to

$$H'=\sum_{i=m}^{n} 2E_3(\theta_{i+1}-\theta_i)\,. \tag{74}$$

(c) *A random distribution of impurities.* At random along the chain there are impurity pendula, pendula with the wrong mass, for which the single particle potential is

$$-\tilde{E}_1\cos\theta_i\,. \tag{75}$$

Since we wish to deal only with the low-field limit, then, from the argument above, we must simply assess the effect of the perturbations on the equilibrium single-particle distribution function. The equilibrium distribution function is calculated using well-known transfer-integral techniques.[6,8,17] As an example, we consider the effect of a perturbation on an otherwise perfect chain of $M+1$ pendula. To illustrate what is involved we calculated the potential-energy part of the partition function, for which we have

$$Z_V=\int d1\cdots d(M+1)e^{\kappa(12)}e^{\kappa(23)}\cdots e^{\tilde{\kappa}(n\,n+1)}\cdots e^{\kappa(M\,M+1)}\delta(\theta_1-\theta_{M+1})\,, \tag{76}$$

where $\kappa(12)=\lambda_1\cos\theta_1+\frac{1}{2}\lambda_2(\theta_2-\theta_1)^2$, $\tilde{\kappa}(n\,n+1)=\lambda_1\cos\theta_n+\lambda_2(\theta_{n+1}-\theta_n-b)^2$, and $b=E_3/E_2$. The δ function in Eq. (76) enforces the periodicity that we require for a simple neutral conducting chain. We note that $\tilde{\kappa}$ is the same as κ except that the spring attempts to create displacement b. Carrying through the standard steps for the TI integration of Eq. (76) we find

$$Z_V=\sum_\nu \langle\phi_\nu(\theta)\,|\,\psi_\nu(\theta+b)\rangle e^{-M\beta\epsilon_\nu}\,, \tag{77}$$

where ψ_ν is an eigenstate of κ, Eq. (62). At low temperatures, a tight-binding representation of $\psi_\nu(\theta)$ leads to ($b=2\pi P+\alpha$, $|\alpha|\ll\pi$)[26]

$$\langle\phi_\nu(\theta)\,|\,\psi_\nu(\theta+b)\rangle=e^{i\nu P}\Omega\,, \tag{78}$$

where

$$\Omega=\int d\theta\,\xi_0(\theta)\chi_0(\theta+\alpha)\,. \tag{79}$$

If the displacement b is small, $P=0$ and the partition function, average displacement of the chain, etc., are unchanged. If $P>0$ the average displacement evolves as shown in Fig. 12, and the chain builds in relative displacement $2\pi P$ between n and $n+1$. In every other regard the chain is unchanged. In particular, the single-particle density is unchanged by the displacement. *Thus, the current carried by the chain is unchanged by the presence of the displacement spring.* The residual displacement α makes no appearance in any of the results. The one-dimensional thermal fluctuations simply wash out any small displacement effects—the chain will accommodate quantized displacements $2\pi P$ with no other changes. These results also obtain for a finite segment of chain with displacement springs (see Fig. 12).

Calculations of the effect of random impurities proceed as illustrated above. For a single impurity at pendulum $m+1$, the kernel in all averages is changed from $\kappa(m\,m+1)$, to

$$\tilde{\kappa}(m\,m+1)=-\tilde{\lambda}_1\cos\theta_m+\tfrac{1}{2}\lambda_2(\theta_{m+1}-\theta_m)^2\,. \tag{80}$$

Using Eqs. (20) and (21) from I we obtain

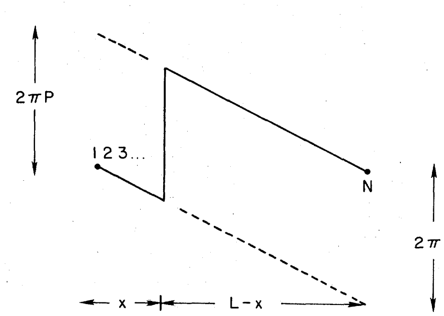

FIG. 12. Equilibrium chain configuration. The equilibrium configuration for a chain with a displacement spring at x is shown. The chain accommodates the displacement spring with minimum phase gradient. Thermal fluctuations in the form of kinks, etc., occur about the average equilibrium configuration. In a weak external field the chain, in the average configuration shown here, is driven down the washboard.

$$\rho(\theta_{n+1}) = \frac{\sum_{\mu\nu} \phi_\nu(\theta_{n+1})\psi_\mu(\theta_{n+1})F_{\mu\nu}e^{-M\beta\epsilon_\nu}\exp[-(n-m)\beta(\epsilon_\nu-\epsilon_\mu)]}{\sum_\nu F_{\nu\nu}\,e^{-M\beta\epsilon_\nu}}, \tag{81}$$

where

$$F_{\mu\nu} = \int d\theta\, \phi_\mu(\theta)e^{\Delta\lambda_1 \cos\theta}\psi_\nu(\theta) = \delta_{\mu\nu}\bar{F}, \tag{82}$$

with

$$\bar{F} = \int d\theta\, \xi_0(\theta)e^{\Delta\lambda_1\cos\theta}\chi_0(\theta) \tag{83}$$

and $\Delta\lambda_1 = \tilde{\lambda}_1 - \lambda_1$. The simple form of the matrix element in Eq. (82) is a consequence of the periodicity of the perturbation; it is the same as the periodicity of $\phi(\theta)$ and $\psi(\theta)$. From Eqs. (81) and (82) we have

$$\rho(\theta_{n+1}) = \phi_0(\theta)\psi_0(\theta),$$

i.e., $\rho(\theta_{n+1})$ is unchanged by the presence of the impurity. Thus the impurity—quite independent of $\tilde{\lambda}_1$—does not effect the current.

In writing Eq. (82) we have taken the ground-state–ground-state matrix element of $F(\theta)$. If we consider matrix elements to the excited states, we can show that there are corrections to $\rho(\theta_{n+1})$ due to the impurity at $m+1$ if $(n-m) \lesssim d$. That is, the impurity exerts an influence proportional to F that decays with distance as $\exp(-|n-m|/d)$. Our conclusion above for a single impurity remains valid until the impurity concentration becomes greater than about d^{-1}.

VII. CONCLUSION

We have calculated the current carried by the sine-Gordon chain in an external field which couples to the phase gradient. The calculation of the current is formulated in terms of the Smolouchowski equation for the configuration-space distribution function—thus, we deal with the chain in the limit of heavy damping. By exploiting the relationship of the Smolouchowski equation to the BBGKY equations and using transfer-integral techniques we are able to find a solution to the SE suitable for calculating the current, Eqs. (57)–(59). Our method of solution for the SE is not specific to the sine-Gordon chain and should prove useful in examining this equation for a variety of nonlinear systems. We find that the conductivity of the chain is linear in the field at low field and at high field, and that these two regimes are separated by a region of highly nonlinear conduction. The region of highly nonlinear conduction occurs when the external field becomes comparable to the single-particle potential of the sine-Gordon chain. The low-field conduction process is due to solitons carrying charge proportional to their phase gradient. The conduction properties of the sine-Gordon chain do not seem to correspond to those observed by Cohen *et al*. for TTF-TCNQ.

We expect the SE treatment of the conduction by the solitons to be valid provided that the external field does not put too much energy into the solitons between collisions, i.e., for

$$dE_0\omega_1\tau \ll k_BT. \tag{84}$$

On the left-hand side we have a product of the factors $E_0\omega_1$ = rate at which the field puts energy into one pendulum, τ = the time between collisions, and d = number of pendula in a soliton. Equation (84) is a statement of the requirement that the energy into the soliton between collisions be small compared to k_BT. A criterion similar to this has been derived by Trullinger from comparison of the results of Fogel *et al*.[5] and of Trullinger *et al*.[9] The validity criterion in Eq. (81) must be comple-

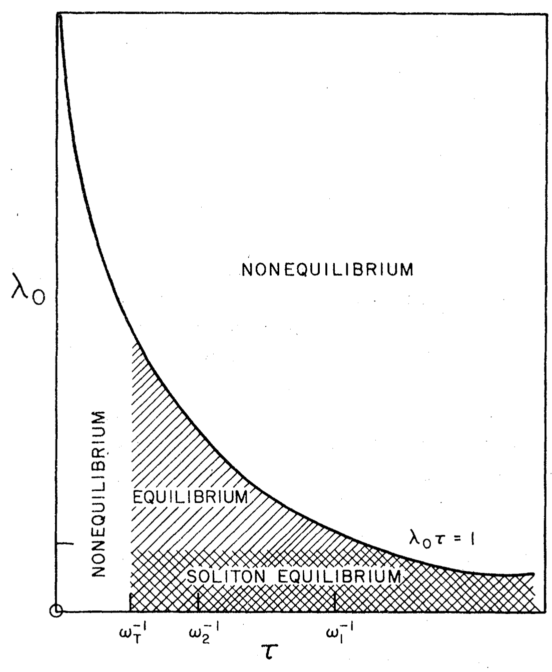

FIG. 13. Validity criterion for the Smolouchowski equation. The solution of the Smolouchowski equation is valid under a variety of circumstances. There are two essential criteria (a) that the frequencies of interest be low compared to the characteristic time τ (this criteria is present even in zero external field), and (b) that the field be such that it doesn't overheat the kinks or the particles, Eqs. (81) and (82).

mented by validity criteria for high field, etc. The SE will satisfactorily describe the motion of a single pendulum (e.g., when $\lambda_2 \to 0$) for $\omega_1\tau \ll 1$. It will satisfactorily describe the motion of the collective modes of the chain for $(\omega_1^2+\omega_2^2)^{1/2}\tau \ll 1$. Finally, at high fields, in place of Eq. (81), we have

$$E_0\omega_T\tau \ll k_B T, \tag{85}$$

where $I\omega_T^2 \approx k_B T$. The SE is valid in the regime shown in Fig. 13.

We have briefly examined the effect of various kinds of perturbations on the current carried by the sine-Gordon chain and a very simple criterion for nonconduction results, Eq. (57). Because of the large one-dimensional fluctuations we expect the chain to wash out the effects of most perturbations.

ACKNOWLEDGMENT

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APPENDIX A: WEAK-COUPLING LIMIT

The self-consistent equation for $e(\theta)$ for case 2, the weak-coupling case, is solved by defining an effective field

$$h(\theta_1) = \lambda_0 - 2\lambda_1 \int d\theta_2\,(\theta_1-\theta_2)\frac{\rho(\theta_1\theta_2)}{\rho(\theta_1)} \times [e(\theta_2)-1], \tag{A1}$$

so that Eq. (40a′) becomes

$$\overline{W}\tau = \rho(1)\left(\frac{\partial e(1)}{\partial 1} + e(1)h(1)\right). \tag{A2}$$

Then, employing an integration procedure like that of Ambegaokar and Halperin, we find

$$e(1) = \overline{W}\tau \exp\int_0^1 [h(1)d1]\left(\frac{1}{\exp\int_0^{2\pi} h(1)d1 - 1} \times \int_0^{2\pi}\frac{d1}{r(1)} + \int_1^{2\pi}\frac{d1}{r(1)}\right), \tag{A3}$$

where $r(1) = \rho(1)\exp\int_0^1 h(1)d1$ and

$$(\overline{W}\tau)^{-1} = \frac{1}{\exp\int_0^{2\pi}h(1)d1 - 1}\int_0^{2\pi} r(1)d1 \int_0^{2\pi}\frac{d1}{r(1)} + \int_0^{2\pi} r(1)d1\int_1^{2\pi}\frac{d1}{r(1)}. \tag{A4}$$

Equations (A1), (A3), and (A4) are a self-consistent set of equations for $e(1)$ and $\overline{W}\tau$. We have employed them to calculate the current when $\lambda_1 \ll \lambda_2$. For the parameters $\lambda_1 = 2.5$, $\lambda_2 = 1.0$ (study 3 of Table I), we found excellent agreement for $\overline{W}\tau$ vs λ_0 between the result obtained using these equations [Eqs. (A1)–(A4)] and the result described in the text using Eqs. (57)–(59).

APPENDIX B: ANALYTIC ASYMPTOTES

The transfer-integral problem is solved in a differential equation approximation as described in I. In low field, the differential equation reduces to the Mathieu equation for which numerous analytic results are available. These analytic results permit us to show $\overline{W}\tau \propto e^{-\beta E_\Phi}$ in low field and provide a number of tests for the numerical work. We display a number of the more useful analytic results here. In low field,

$$\psi_0(\theta) = ce_0[\tfrac{1}{2}(\pi+\theta); q],$$

$$\phi_0(\theta) = e^{-\lambda_1\cos\theta}\psi_0(\theta),$$

$$\rho(\theta) = \phi_0(\theta)\psi_0(\theta),$$

$$\theta\to 0;\ \psi_0(\theta) = [(\sqrt{q}-\lambda_1)/2\pi]^{1/4}e^{\lambda_1/2}e^{-\sqrt{q}\theta^2/4}, \tag{B1}$$

$$\rho(\theta) = [(\sqrt{q}-\lambda_1)/2\pi]^{1/2}\exp[-(\sqrt{q}-\lambda_1)]\tfrac{1}{2}\theta^2, \tag{B2}$$

$$\theta\to\pi;\quad \psi_0(\theta) \approx ce_0(0;q)\cosh\sqrt{q}(\theta-\pi), \tag{B3}$$

$$\rho(\theta) \approx 8\left(\frac{\sqrt{q}-\lambda_1}{2\pi}\right)^{1/2}\exp[2\lambda_1 - 2\sqrt{q} - \tfrac{1}{2}\lambda_1(\theta-\pi)^2] \times \cosh^2\sqrt{q}(\theta-\pi). \tag{B4}$$

It is $\rho(\theta)$ given by Eq. (B4) that is used to produce the analytic asymptotes, shown by dashed lines in Fig. 6, against which the numerical work was checked. It is also Eq. (B4) in the limit $\lambda_1 \to 0$, $\lambda_1\lambda_2 \to q$ that gives $\rho(\pi) \propto e^{-\beta E_\Phi}$, i.e., conductivity due to the continuum soliton.

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[1]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1974).

[2]A. D. Bruce, Ferroelectrics 12, 21 (1976).

[3]J. A. Krumhansl, Sanibel Symposia (1977) (unpublished).

[4]M. J. Rice, A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Phys. Rev. Lett. 36, 432 (1976).

[5]M. B. Fogel, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. Lett. 36, 1411 (1976).

[6]N. Gupta and B. Sutherland, Phys. Rev. A 14, 1790 (1976).

[7]J. F. Currie, M. B. Fogel, and F. Palmer, Phys. Rev. A 16, 796 (1977).

[8]R. A. Guyer and M. D. Miller, Phys. Rev. A 17, 1205 (1978) (thereafter this paper is referred to as I).

[9]A preliminary report of some of the work described here has been submitted for publication jointly with Trullinger and co-workers.

[10]We use the words *kink* and *soliton* interchangeably. In the continuum limit (as the kink occurs over many units) there is a known soliton solution to the equation

of motion for θ. This solution is given in Eq. (5) and discussed in detail in Ref. 11. Most of the results on the sine-Gordon chain are obtained in the continuum limit. The theory we develop here is valid for the discrete chain and is able to be taken to the continuum limit. We expect qualitative phenomena, found in the continuum limit (Refs. 11–13) to also occur on the discrete chain. We use the word kink in preference to the word soliton as a reminder that we are describing a discrete chain.

[11]A. C. Scott, F. Y. E. Chu, and D. W. McLaughlin, Proc. IEEE 61, 1443 (1973).

[12]K. Nakajima, T. Yamashita, and Y. Onodera, J. Appl. Phys. 45, 3141 (1974).

[13]In agreement with the discussion of Ref. 1; see Ref. 11.

[14]M. J. Rice, in *One Dimensional Conductors, GPS Summer School Proceedings* (Springer-Verlag, New York, 1975).

[15]This model of the sine-Gordon chain was suggested to us by T. R. Koehler who attests to its usefulness.

[16]The Smolouchowski equation for the sine-Gordon chain has been derived by S. E. Trullinger in the context of a discussion of charge-density waves; S. E. Trullinger and co-workers (to be published).

[17]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. B 6, 3409 (1972); the equilibrium one, two, ... densities can be found using the methods described in this paper. See Ref. 8 for the application of these methods to the discrete chain.

[18]V. Ambegaokar and B. I. Halperin, Phys. Rev. Lett. 22, 1364 (1969).

[19]F. Roig, M. D. Miller, and R. A. Guyer (unpublished).

[20]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (U.S. Department of Commerce, Washington, D.C., 1970).

[21]When $E_0 \neq 0$ and the ends of the chain are unpinned, the chain is not in statistical equilibrium, there are currents, ... In this circumstance, a kink creation energy has intuitive meaning although it is not well defined.

[22]Here we use the word soliton to describe the smooth evolution of phase over several units of the chain (see Ref. 11).

[23]See Ref. 8.

[24]M. J. Cohen, P. R. Newman, and A. J. Heeger, Phys. Rev. Lett. 37, 1500 (1976).

[25]W. Wonneberger and F. Gleisberg, Solid State Commun. 23, 665 (1977).

[26]This restriction is not necessary but it makes the discussion a good deal simpler. For details of the tight binding approximation, see Ref. 8, Appendix C.