Low-temperature dynamics of sine-Gordon solitons

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We examine the theory of a kink's random walk in the classical sine-Gordon continuum at temperatures much lower than the kink's rest energy. The description of the thermal bath in terms of phonons or breathers is shown to yield identical results for the diffusion constant, provided the underlying thermodynamic fluctuations are properly taken into account. We present molecular-dynamics evidence for the occurrence of the soliton-diffusion phenomenon and discuss the relevance of intrinsic discretization effects to numerical and experimental data.

I. INTRODUCTION

The sine-Gordon (SG) model has been of considerable importance in the study of nonlinear phenomena. Its classical continuum version is a prototype of a completely integrable Hamiltonian system capable of supporting kink- or breatherlike solitonic excitations. A variety of real systems quite distinct in their physical origins—such as Josephson junctions, charge-density waves, and one-dimensional magnets—possess salient features which can be described by the SG Hamiltonian.

Recent neutron spin-echo experiments[1,2] with the one-dimensional antiferromagnet $(CD_3)_4NMnCl_3$ (TMMC) have revealed signatures of diffusive dynamics. At temperatures T much lower than the kink rest energy E_0 interactions between kinks are expected to be negligible and the resulting single-kink dynamics should be dominated by collisions with the low-energy excitations which constitute the heat bath. Early theories[3–5] based on a phonon picture of the thermal bath had predicted a kink diffusion constant proportional to T^2. More recently an alternative description in terms of breathers[6] led to a similar result, albeit with a different prefactor. The slight disagreement was attributed by the authors of Ref. 6 to the different underlying statistical properties of phonons and breathers, respectively.

The discrepancy between the breather and phonon formulations of the same phenomenon within a classical, continuum, low-temperature approximation, i.e., in a regime where the two descriptions have until now yielded identical results,[7] presents an interesting challenge to our theoretical understanding of SG dynamics. If the results of Refs. 3 and 6 are both correct in their respective contexts, we might obtain the means of identifying the "true" character of low-energy excitations by performing an appropriate low-temperature experiment or a numerical simulation; this would resolve the apparent phonon-breather dilemma.[7] On the other hand, a careful consideration of the development of equilibrium statistical mechanics of solitons shows that until recently a theory of thermodynamic fluctuations, essential for the construction of dynamical phenomenologies and/or soliton kinetics, had not been formulated.[8] One of the basic findings of Ref. 8 (to be referred to as I in the rest of this paper) is that *small-amplitude breathers do not even approximately obey Maxwell-Boltzmann statistics.* Since both approaches (phonon,[3] as well as breather,[6] based) make implicit use of the classical limit of statistical fluctuations, we feel that a reexamination of soliton diffusion theory might prove useful.

The purpose of this work is accordingly twofold. First we present a brief derivation of the soliton diffusion constant, taking the results of equilibrium fluctuation theory as developed in I fully into account. We thus demonstrate that both descriptions of the heat bath, i.e., in terms of phonons or breathers lead to *identical* results. The phonon-breather duality apparently persists beyond thermodynamics—at least within the confines of classical continuum theory as applied to the low-temperature regime.

Our second aim has been to attempt a direct observation of soliton diffusion using a molecular-dynamics simulation. Rather than evaluate the structure factor and analyze it in terms of all possible competing scattering processes, we have chosen to follow the motion of a single kink in real time. Our approach emphasizes the microscopic dynamics and should be regarded as complementary to the structure factor studies.[9,10] Regarding the particular issue of spin diffusion the concept is, in principle, straightforward. If the individual-kink dynamics is governed by elastic interactions with the heat bath, as suggested by continuum SG theory, the kink should have a constant average velocity over a long enough period of time. By subtracting this uniform part of the motion and taking the time average of the square of what is left we should be able to detect any signature of diffusive behavior and extract the corresponding diffusion constant. Our numerical results suggest that things may not be that simple.

The problem we encounter within the context of (in-

herently discrete) molecular dynamics is that although "primary" effects of the lattice (e.g., pinning) can be eliminated by an appropriate choice of lattice constant,[11] "secondary" effects persist. There is simply no way to eliminate the *existence* of slow zone-edge phonons from a numerical simulation. It has been known for some time[12] that these phonons lead to inelastic scattering processes and may in fact provide the necessary channel for thermalization. Our numerical results underline the qualitative importance of such effects and, at least to some extent, serve to quantify them.

We have been able to detect soliton diffusion by artificially suppressing zone-edge phonons—thus indirectly attesting to the latter's practical significance. The results obtained are in agreement with the predictions of continuum theory. However, in view of the crucial role played by phonons near the Brillouin-zone edge in providing a channel for the exchange of kinetic energy, we have undertaken a systematic study of the fundamental inelastic scattering process involved. The numerical results suggest that the only relevant parameter is the relative velocity of the phonon relative to the kink and can be well described by analytical expressions derived within second-order perturbation theory. On the basis of our findings, we can give a rough theoretical estimate of the time needed for the nearly integrable discretized version of the SG system to reach thermal equilibrium. As expected, this time increases as the discretization becomes finer and the temperature drops.

The qualitative picture which emerges from our numerical work can be summarized as follows. At very long times inelastic processes inherent to any discretization procedure may result in a *dissipative* (conventional) Brownian motion. From the experimental point of view such time scales are probably irrelevant as long as the spatial extent of the kink substantially exceeds the lattice constant (although other *extrinsic* dissipative mechanisms with similar formal structure, such as impurities, may have measurable consequences). Intermediate time scales are characterized by free (ballistic) kink motion, and only at even shorter time scales does the *nondissipative* (anomalous[6]) diffusion dominate the dynamics. The anomalous diffusion component would naturally reveal itself in the high-frequency part of the dynamic structure factor.[3,6] Its detection via our "straightforward" real-time numerical procedure sets too-high demands on the system's degree of integrability. In this sense the "filtering out" of zone-edge phonons is not as arbitrary as it might seem at first glance; by suppressing zone-edge phonons it "simulates the continuum;" by eliminating processes with extremely long time scales it produces a random walk pattern which is *per se* artificial—yet its diffusion constant is in fact the one that would be detected in an experiment with a finite frequency resolution. We thus hope that the real-time approach, once its limitations are properly assessed, will contribute to the understanding of both soliton diffusion *and* inherent discretization effects.

The paper is organized as follows. In the next section we demonstrate the equivalence of the phonon and breather approach to continuum kink diffusion. Section III deals with the molecular dynamics of diffusion, Sec. IV with the effects of zone-edge phonons. Some concluding remarks can be found in Sec. V. Calculational details of the theoretical part have been reserved for the Appendix.

II. A KINK'S RANDOM WALK IN THE SG CONTINUUM

We consider the SG equation in the form

$$\ddot{\phi}=c_0^2\phi_{xx}-\omega_0^2\sin\phi\ , \tag{1}$$

where the parameters c_0 and ω_0 represent the limiting velocity and phonon gap frequency, respectively. The kink width is then given by $d=c_0/\omega_0$. The basic physical mechanism underlying the soliton dynamics of (1) at low temperatures—beyond free propagation—is the elastic scattering which occurs during a kink-phonon or a kink-breather collision. Such a scattering process is elastic, i.e., it gives rise only to a spatial shift of the colliding partners without changing their velocities; at zero temperature, the resulting evolution of any initial configuration can be predicted by inverse scattering theory. At finite temperatures, such an exact description is not possible. However, we mention parenthetically that an interesting perturbation theoretical approach developed by Kaup and Osman[13] primarily for the purpose of describing the damped SG system should, in principle, describe the conservative system (1) in the limit of zero damping—although this remains to be verified to second (i.e., leading nontrivial) order in T.

It is important to realize that the actual mechanism of thermalization is left out of consideration in the present discussion. Clearly in a real system effects extrinsic to (1), such as discretization or impurity damping, are crucial in establishing thermal equilibrium and may, depending on the exact circumstances, have more or less serious consequences for the dynamics. In this section we will consider the heat bath as a fact, i.e., a canonical ensemble average over all possible realizations of the completely integrable system (1); accordingly we will operate within the strict context of continuum SG dynamics and statistical mechanics; the diffusive dynamics of a single kink placed in such a heat bath arises in a nondissipative fashion as a random walk due to a series of spatial shifts $\{\Delta(k)\}$ of the kink, brought about by a stochastic sequence of independent collisions with low-energy excitations of type $\{k\}$. An illustration of the fundamental microscopic event is given in Fig. 1.

The assumption of independent collisions presents some problems even within the strict context of continuum SG theory. At low temperatures the constituents of the heat bath—whether we like to think of them as phonons or as breathers—become more and more extended, and might thus be characterized by a significant overlap. We will return to this point in Sec. IV and present some evidence supporting the hypothesis of statistical independence.

Within the general framework outlined an elementary kinetic theory of soliton diffusion can be presented as follows.[3(b)] Under the influence of $n_\tau(k)$ collisions with

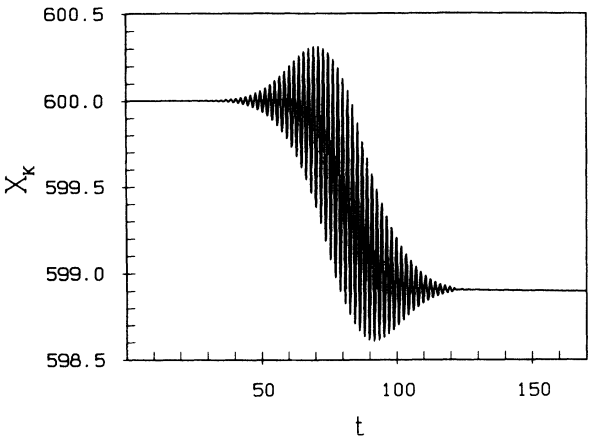

FIG. 1. Kink position during a collision of an initially resting kink with a wave packet composed of relatively long-wavelength phonons ($q=0.2\pi$). The kink comes completely to rest after the collision; the only asymptotic effect is a spatial shift.

each heat bath constituent of type k, the position of a kink which is initially at rest at the origin evolves within the time τ according to

$$X(\tau)=\sum_k \Delta(k)n_\tau(k) \ . \tag{2}$$

Note that we still reserve our option to specify the actual type of excitation $\{k\}$ giving rise to the random-walk process (2). It is possible to convert the sum (2) into an integral by introducing the appropriate density of states function $R(k)$; at this stage R is a function of the particular configuration of our heat bath (cf. I). The product function $\rho_\tau(k)=R(k)n_\tau(k)$ is a further useful quantity. In the context of our elementary kinetic arguments $\rho_\tau(k)dk$ represents the number of times the kink collides with heat-bath constituents lying between k and $k+dk$. The integral form

$$X(\tau)=\int dk\ \Delta(k)\rho_\tau(k) \tag{2'}$$

allows us to write down directly an expression for the fluctuations with respect to (w.r.t.) the thermal average of $X(\tau)$

$$\delta X(\tau)=\int dk\ \Delta(k)\delta\rho_\tau(k) \ , \tag{3}$$

in terms of the deviations of the configuration $\{n(k)\}$ from its value at thermal equilibrium. Note that for our particular choice of initial condition, i.e., a kink resting at the origin, the thermal average $\langle X(\tau)\rangle$ vanishes. The quantity we are interested in is the variance

$$\langle[\delta X(\tau)]^2\rangle=\int dk\,dk'\,\Delta(k)\Delta(k')\langle\delta\rho_\tau(k)\delta\rho_\tau(k')\rangle \ . \tag{4}$$

If diffusive behavior actually occurs, the right-hand side (rhs) of (4) should be proportional to τ; the proportionally constant can then be identified with $2D$, where D is the kink diffusion constant.

At this point we face the traditional breather versus phonon dilemma. In order to illustrate the relevance of the underlying theory of thermodynamic fluctuations it will be useful to outline both the harmonic phonon and the small-amplitude breather versions.

A. Harmonic phonons

The density of states is $R_0(k)=R_0=L/2\pi$ and the relevant fluctuations entering (4) are

$$\langle\delta\rho_\tau(q)\delta\rho_\tau(q')\rangle=\frac{|v(q)|\tau}{L}\langle\delta\rho(q)\delta\rho(q')\rangle \tag{5a}$$

$$=\frac{v(q)|\tau}{L}R_0\delta(q-q')\langle[\delta n(q)]^2\rangle \ , \tag{5b}$$

where $v(q)$ is the group velocity of phonons with wave vector q. Using (i) the continuum SG dispersion relation

$$\omega^2(q)=\omega_0^2+c_0^2q^2 \ , \tag{6}$$

(ii) the classical limit of Bose-Einstein statistics

$$\langle[\delta n(q)]^2\rangle=\left[\frac{1}{\beta E(q)}\right]^2 \ , \tag{7}$$

where $E(q)$ is the energy of a phonon, and (iii) the known expressions for the kink phase shift

$$\Delta(q)=\frac{E(q)}{E_0}\frac{2d}{1+d^2q^2} \ , \tag{8}$$

it can be shown that the rhs of (4) is indeed equal to $2D_{\rm ph}\tau$, where the diffusion constant

$$D_{\rm ph}=\int\frac{dq}{2\pi}|v(q)|\left[\frac{\Delta(q)}{\beta(E)q}\right]^2$$

$$=2\bar{T}^2d^2\omega_0^4\int\frac{dq}{2\pi}\frac{|v(q)|}{\omega^4(q)}$$

$$=2\bar{T}^2d^2\omega_0^4\int\frac{dq}{2\pi}I_D(q)$$

$$=\frac{C}{3\pi}\frac{c_0^2}{\omega_0}\bar{T}^2 \tag{9}$$

is expressed in terms of the dimensionless temperature $\bar{T}=k_BT/E_0$. The integrand I_D is shown in Fig. 6 and compared to its discrete lattice counterpart (cf. the discussion in Sec. IV).

B. Breathers

In order to characterize the SG breather we must specify its rapidity α, which fixes the canonical velocity $v(\alpha)=c_0\tanh\alpha$ and a parameter θ $(0\le\theta<\pi/2)$, which defines the internal frequency of oscillation $\omega=\omega_0\cos\theta$. Although breathers remain strongly interacting objects even at low temperatures (since their total number is $N/2$ in a chain of N particles[7] there is no dilute limit of the breather gas) an important simplification does occur in the harmonic (low-temperature) limit: Interactions are

diagonal in the α subspace, hence only breathers with the same velocity give rise to mutual phase shifts. This has important consequences for thermodynamic fluctuations as well as for our simple kinetic argument underlying (5). The "breather alternative" of (5a) is given by

$$\langle \delta\rho(\alpha,\theta)\delta\rho(\alpha',\theta')\rangle_\tau = \frac{|v(\alpha)|\tau}{L}\langle \delta\rho(\alpha,\theta)\delta\rho(\alpha',\theta')\rangle \ . \tag{10}$$

The linear dependence on τ provides again the signature of diffusive behavior. Note, however, that in this case we cannot claim a constant density of states R. The correlation function in the rhs of (10) can be formally expressed in terms of the elementary breather-breather phase shifts as [cf. Eq. (28) of I]

$$\langle \delta\rho(k)\delta\rho(k')\rangle = \int dk''\,\bar{\rho}(k'')\bar{B}(k,k'')\bar{B}(k',k'') \ , \tag{11}$$

where $k=(\alpha,\theta)$, and the function $\bar{B}(k',k'')$ contains information about phase shifts and occupation numbers of all breather modes; due to the diagonal property of the breather-breather phase shifts in the α subspace[7] $\bar{B}$—and hence the correlation function on the rhs of (10)—is proportional to $\delta(\alpha-\alpha')$. The bars indicate that the corresponding quantities are to be evaluated at thermal equilibrium. For details the reader is referred to I. For our purposes it is sufficient to point out that the hypothesis of Maxwell-Boltzmann statistics for breathers is equivalent to setting $\bar{B}$ equal to a δ function in both α and θ subspaces and yields the wrong specific heat.

We now introduce the elementary steps of the random walk, i.e., the kink shift due to its interaction with a single breather

$$\Delta(\alpha,\theta)=2d\frac{E(\alpha,\theta)}{E_0\cosh^2\alpha} \ , \tag{12}$$

where

$$E(\alpha,\theta)=2E_0\sin\theta\cosh\alpha$$

is the breather energy, and obtain

$$D_{\rm br}=\frac{2d^2}{E_0^2L}\int d\alpha\frac{|v(\alpha)|}{\cosh^4\alpha}\int\int\int\int\int d\alpha'\,d\alpha''\,d\theta\,d\theta'\,d\theta''\,\bar{\rho}(\alpha,\theta)E(\alpha',\theta')E(\alpha'',\theta'')\bar{B}(\alpha',\theta';\alpha,\theta)\bar{B}(\alpha'',\theta'';\alpha,\theta) \ . \tag{13}$$

The quintuple integral in the rhs of (13) looks rather complicated, especially since the explicit form of $\bar{B}$ is not known. However, as may be readily guessed by a comparison with (11) and confirmed by Eq. (36) of I, provided $\bar{B}$ is diagonal in the α subspace (which is exactly the case at low temperatures), this integral is closely related to energy fluctuations, i.e., to the specific heat associated with a mode of a given rapidity α. Its exact value is

$$I(\alpha)=\bar{T}^2L\cosh\alpha/2\pi d \ .$$

Details of the evaluation are given in the Appendix. The resulting expression

$$D_{\rm br}=2\bar{T}^2c_0d\int\frac{d\alpha}{2\pi}\frac{|\tanh\alpha|}{\cosh^3\alpha} \tag{14}$$

coincides with the second line of (9) if we identify $qd=\sinh\alpha$.

This completes the demonstration of the breather-phonon equivalence as far as their respective effects on kink diffusion are concerned. The fact that $D_{\rm br}=D_{\rm ph}$ implies that it is not possible to exploit the soliton diffusion phenomenon in order to determine the consistency of our heat bath. Any distribution function which describes the specific heat correctly will yield the same diffusion constant. Conversely, a theoretical description of kink diffusion which yields values different from (9) in the classical, continuum, low-temperature regime fails to describe the underlying thermodynamic fluctuations properly.

III. MOLECULAR DYNAMICS

The discretized form of (1)

$$\ddot{\phi}_l=c_0^2(\phi_{l+1}+\phi_{l-1}-2\phi_l)-\omega_0^2\sin\phi_l \tag{15}$$

is integrated subject to the boundary condition

$$\phi_{N+l}=\phi_l+2\pi \tag{16}$$

for a chain of $N=1000$ particles using the Verlet[14] algorithm with a time step $\Delta t=0.01$. We have taken the parameter values $c_0^2=29.22$ and $\omega_0=1$. Time is thus measured in units of $1/\omega_0$ and distances in multiples of the lattice constant. Thermalization is produced by Langevin forces following the example of Schneider and Stoll.[9,15] The reader is referred to their work for details. The form of the boundary condition guarantees the existence of an odd number of kinks and/or antikinks; in the temperature range of interest in this work this practically restricts us to single-kink configurations and thus facilitates the task of detecting the kink's position defined by the value of the displacement field $\phi=\pi$. The fast oscillations of the kink position during the course of a collision event (Fig. 1) can be eliminated by appropriate averaging.

In order to study the nondissipative time evolution of the kink's position we turned off the Langevin forces after achieving thermalization. Contrary to what one would expect from the continuum SG model (cf. our discussion in the previous section) the kink does not propagate with a constant average velocity over long periods of time (Fig. 2). We have attributed this property to the de-

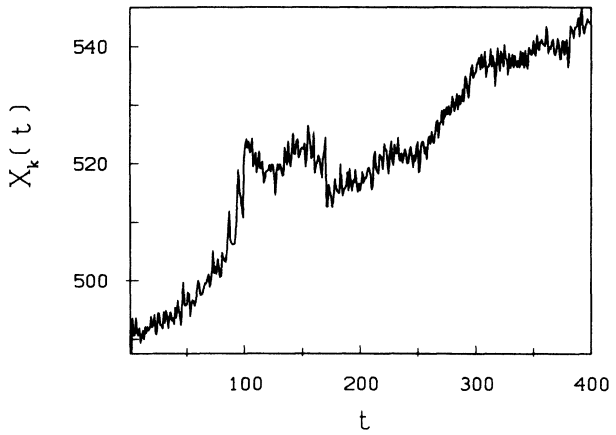

FIG. 2. The trajectory of a kink injected into a SG lattice at a reduced temperature $\bar{T}=0.15$, followed for approximately 400 time units. Although the typical time scale involved in inelastic scattering processes is smaller than the observation time, it is apparently not short enough to bring out a thermalization of the kink (defined by demanding that the time average of the velocity should be equal to zero). Thus although the kink fails to meet the strict demands of continuum SG theory, it cannot be treated as the usual Brownian particle at these finite time scales.

viations of the discrete version (15) from its completely integrable continuous counterpart (1). The microscopic mechanism behind the change in (canonical) velocity has been investigated long ago[12] and was shown to be related to interactions with zone-edge phonons, for which an illustrating example can be seen in Fig. 3. We will present some additional results concerning this point in the next section. For present use, being interested in simulating the continuum we apply the following technique in order to *eliminate* the influence of such effects inherent to the discretization procedure. At distances far from the kink ($\geq 8d$) we produce a thermal bath via the usual Langevin algorithm. In the vicinity of the kink we turn off the random force while retaining the small friction of the Langevin extensions of (15). Strictly speaking the average energy of our system is thus not quite constant, since a small portion of the chain violates the fluctuation-dissipation theorem. The small energy losses, however, come mainly from the damping of slow zone-edge phonons which are dissipated before they reach the kink. The small friction ($\Gamma=0.02$ in our dimensionless units) is not enough to damp out faster excitations, which reach the kink, contribute to its random-walk dynamics, and are then "regenerated" by the Langevin forces which are still active far from the kink. The regeneration is a major advantage of the Langevin molecular-dynamics formalism[9] versus the pure Newton's equations (15), since it circumvents the recurrence problem which would start to occur in our chain after $1000/c_0 \approx 185$ time units, i.e., well within our time scale of observation.

We believe that this somewhat unconventional procedure allows us to unmask the basic features of continuum SG dynamics. At the same time, the fact that we have to resort to such means underlines the significance of intrinsic discretization effects—at least over the relatively long time scales needed to perform a reliable statistical averaging of our data.

We have followed the time evolution of a kink initially at rest for approximately 10^5 time steps, averaged the square of the fluctuation of its position, and obtained the results shown in Fig. 4 exemplarily for the case $\bar{T}=0.1$. The pattern of the motion is manifestly diffusive at least up to times of the order $1/\Gamma$ and allows us to extract the value of the diffusion constant. We have repeated the numerical experiment at five different temperatures and obtained the temperature dependence of the diffusion constant shown in Fig. 5. The parameter-free fit to (9) provides a convincing demonstration of the theoretical framework presented in Sec. II *within its original context, i.e., the continuum low-T limit.* At the same time the limitations of the theory, if it is to be applied to any real

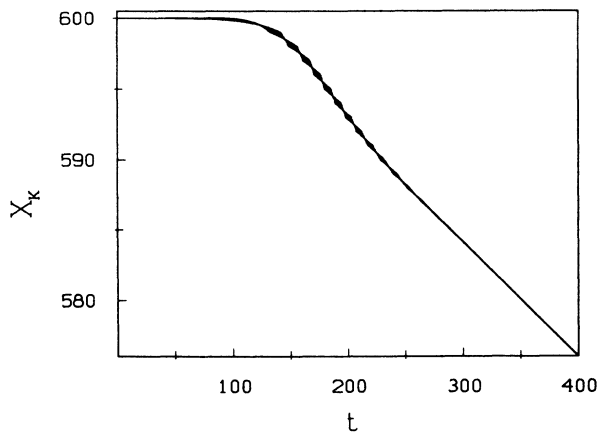

FIG. 3. Kink position during a collision of an initially resting kink with a wave packet composed of near zone-edge phonons ($q=0.9\pi$). The kink does not come to rest after the collision, but suffers in addition to the spatial shift a velocity shift. This should be contrasted to the collision with a continuumlike phonon as in Fig. 1.

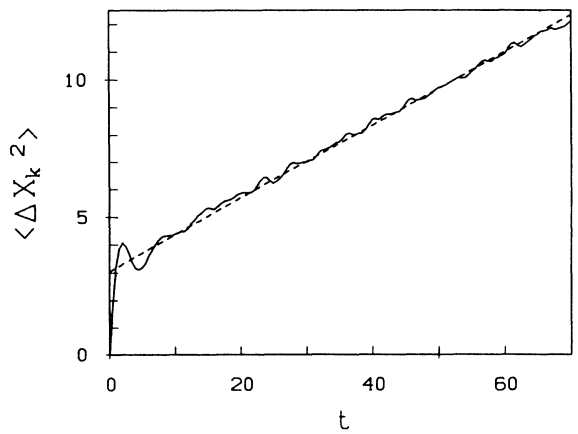

FIG. 4. The plot of the averaged fluctuation in kink position $\langle \Delta X_k^2 \rangle$ vs time t for $\bar{T}=0.1$ exhibits manifestly diffusive behavior after the suppression of slow phonons. The dashed line is a linear fit, the slope being two times the diffusion constant.

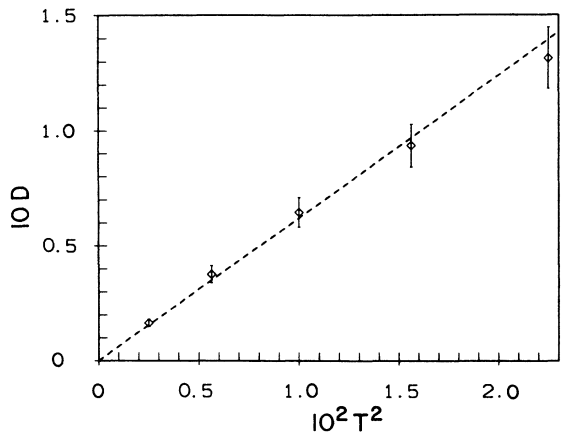

FIG. 5. Temperature dependence of the kink diffusion constant. Numerical results are shown for five different temperatures along with error bars assuming a 10% uncertainty. The dashed line represents the predictions of continuum theory based on either the phonon (9) or the breather (14) picture.

discrete system, become apparent. The ideal nondissipative diffusive-kink motion envisaged in Refs. 3–6 was observed over long time intervals only after artificial suppression of zone-edge phonons.

In Sec. IV we will present some additional results on the subject of zone-edge phonons. This should help us assess both the fundamental significance of residual discretization effects and their actual impact on observable dynamics.

IV. RESIDUAL (INTRINSIC) EFFECTS OF DISCRETIZATION

It has been recognized for a long time that whereas some physical effects of the lattice, such as the Peierls barrier, or its influence on certain thermodynamic properties of solitons may be eliminated by decreasing the lattice constant a, others persist even in the limit $d/a \gg 1$, being intrinsic to the discretization procedure. There is no *a priori* reason why the collision of a kink with a lattice phonon of arbitrary wave vector should be elastic. It turns out[12] that for both ϕ^4 and SG models the majority of collision events maintain their elastic property to second order in the phonon amplitude, although the numerical values of the phase shifts deviate appreciably from those obtained in the continuum limit. Furthermore, a small minority of phonons (from the immediate vicinity of the zone edge) gives rise to inelastic scattering (cf. Fig. 3).

There are, therefore, two possible intrinsic effects of discretization which we have to discuss. We begin with the simplest. Even if we neglect inelastic scattering events, in view of the substantial deviations of the discrete phonon phase shifts from their continuum counterparts, to what extent can we regard the numerical value of the diffusion constant obtained by the continuum formalism as reliable? To obtain a reasonable estimate we must look at the integrand I_D in (9), rather than the individual phase shifts. The presence of the velocity factor in I_D suggests that the slower discrete phonons, in spite of the larger phase shifts they cause, may not contribute decisively to the diffusion constant. This is verified in detail in Fig. 6, which demonstrates that the dominant contributions come from a relatively narrow band of long-wavelength ($q \sim 0.05\pi$) phonons. Thus we may reasonably expect continuum theory to yield a correct numerical value of D.

Returning to the issue of the independence of collision events raised in Sec. II, we conclude from a comparison of Figs. 6 and 7 that the phonons which actually contribute to the diffusion process are relatively fast. A relatively narrow band of fast-collision partners is not expected to lead to significant overlap and the assumption of statistical independence seems justified.

We now proceed to discuss inelastic scattering events. Perturbation-theoretical calculations[12] and preliminary numerical results[16] have indicated that a kink which is initially at rest may acquire kinetic energy by colliding with a near zone-edge phonon. We have extended the scope of our numerical work to include moving kinks; our findings suggest, in accordance with the Galilean invariance of (15) that (as long as relativistic corrections can be neglected) the only relevant parameter for the kink's velocity change Δv is the relative velocity of kink and phonon $v_{\rm rel} = v(q) - v$ prior to the collision event. In Fig. 8 we plot the velocity change against the initial relative velocity for various configurations of initially static or moving kinks. The corresponding expression obtained in second-order perturbation theory is

$$\Delta v = -2v_{\rm rel}\frac{E(q)}{E_0}\left[1+\frac{\sinh^2(2\pi v_{\rm rel})}{\cosh^2\pi\sqrt{7}/2}\right]^{-1} . \qquad (17)$$

This relation implicitly assumes a constant $v_{\rm rel}$ during a

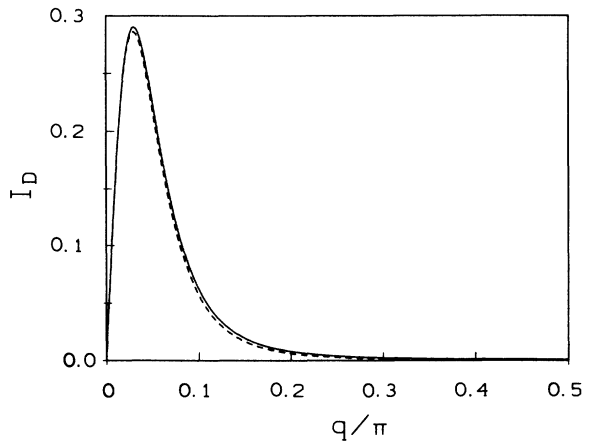

FIG. 6. The diffusion integral $I_D(q)$, as defined in (9), determines the contribution of any given phonon mode to the diffusion constant. The dominant contribution arises from a relatively narrow band of long-wavelength phonons. Furthermore, due to the compensating presence of the velocity factor (cf. Fig. 7), continuum theory (---) agrees quite well with the results for the discrete lattice (——).

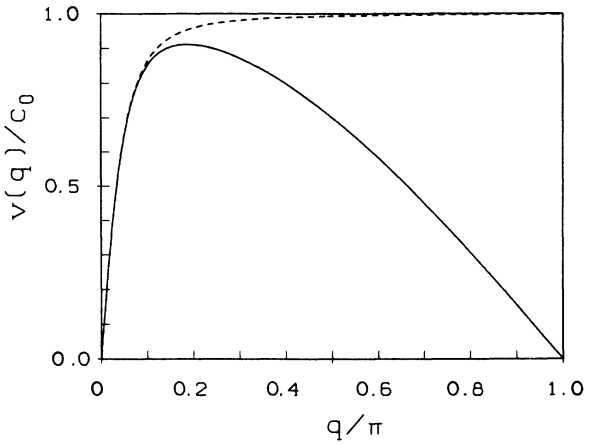

FIG. 7. Phonon group velocity v vs q. Lattice phonons (——) are slower than their continuum counterparts (---). The decisive contribution to the diffusion phenomenon, however, comes from phonons with a wave vector of the order of 0.05π, which can be well approximated by continuum theory.

collision, i.e., $\Delta v \ll v_{\rm rel}$. To fit the numerical data in Fig. 8 one has to take into account corrections to this idealization. The numerical data are well fitted by substituting $v_{\rm rel}$ in the rhs of (17) by $v_{\rm rel}+\Delta v/2$ (i.e., the arithmetic mean of initial and final relative velocity) and then determining Δv self-consistently.

The inelastic scattering event described above provides the only mechanism—except for boundary or finite-site

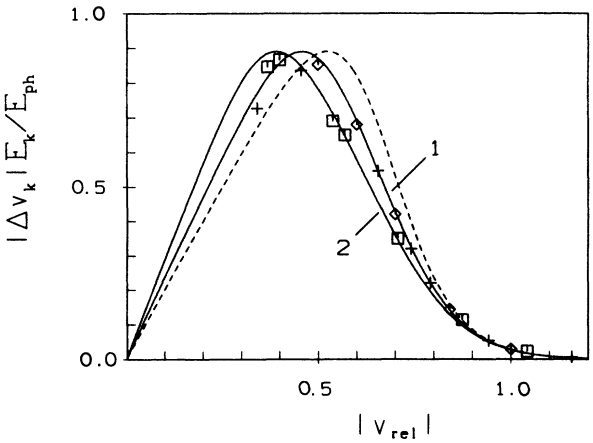

FIG. 8. Change Δv_k in the kink velocity as a result of a kink-phonon wave-packet collision. As described in the text, after taking into account corrections to the bare theory (17) (dashed line) the numerical results are well fitted by the theoretical prediction. Curve 1 is for $E_{\rm ph}/E_k=0.15$, + are the numerical results for different initial kink velocities, ◇ that for different wave vectors, i.e., group velocities, of the colliding phonon. Curve 2 is for $E_{\rm ph}/E_k=0.3$, □ are the corresponding numerical results for different phonon wave vectors. This demonstrates, that as long as the phonon energy $E_{\rm ph}$ is much lower than the kink energy E_k and relativistic effects are negligible, the (initial) relative velocity $v_{\rm rel}$ of kink and phonon is the only relevant parameter.

effects—that can lead to a change in the state of motion of a kink in the almost integrable system (15). Thus its importance extends beyond, in fact mainly beyond, the issue of soliton diffusion and into the fundamental question of *how* and *after how long* small deviations from complete integrability can bring about thermal equilibrium. As a first step one might use a simple kinetic-theory argument similar to the one presented in Sec. II, where now the microscopic input is the shift in the kink's velocity (17) rather than in its position. This leads to a conventional (dissipative) Brownian motion with a typical thermalization time $\tau_{\rm th}$ (given by the inverse of the friction constant γ) of the order of $\omega_0^{-1}\bar{T}^{-1}(d/a)^3$. At very long times $t>\tau_{\rm th}$, as the kink loses memory of its initial velocity, this implies a temperature-independent diffusion constant of the order $D_0\sim c_0^2\omega_0^{-1}(d/a)^3$.

This diffusion constant is several orders of magnitude larger than (9). Its relevance, however, is restricted to the extremely long time scales necessary for thermalization of the almost integrable system (15). In a system with $d/a\gg 1$, the features of the dynamical structure factor determined at low temperatures and with finite frequency resolution will reflect (9) in the high-frequency tail.[3,6] Any influence of the Brownian particlelike behavior would be restricted to an undetectably narrow region around $\omega=0$.

Although our numerical simulations are consistent with the rough estimate of the thermalization time $\tau_{\rm th}$ above (resulting in $\tau_{\rm th}\sim 1000/\omega_0$ for our simulation parameters $d/a=5.4$ and $\bar{T}=0.15$) in the sense that significant changes of the kink velocity occur in time intervals of that order, a quantitative verification of the thermalization process and the associated diffusion constant D_0 would by far exceed our computational capacities.

It is, however, worth noting that for our type of system, where d/a is much larger than unity, the power-law behavior of $\tau_{\rm th}$ leads to small but observable consequences (even if we neglect other thermal forces) as opposed to what one would expect from the exponentially vanishing lattice friction.[17]

V. CONCLUDING REMARKS

We have shown that the random walk of a kink in the SG continuum chain can be described in identical fashion for both versions of the small amplitude constituents of the continuum heat bath. Breather[6] and phonon[3] descriptions of the heat bath lead to the same kink diffusion constant, provided the underlying thermodynamic fluctuations are fully incorporated into the theory. The persistence of phonon-breather duality in the context of a *dynamical* phenomenon suggests that it may prove extremely difficult to determine the true consistency of a finite-temperature SG chain.[7,8]

Our numerical simulation confirms the validity of continuum theory insofar as it reveals diffusive kink behavior at short time scales after the filtering out of inelastic processes due to zone-edge phonons. The diffusion constant extracted is in full agreement with the predictions of continuum theory.

On the basis of our numerical results it is possible to assess the qualitative and quantitative importance of residual discretization effects. The qualitative significance lies in the fact that discretization—with the ensuing inelastic scattering processes—provides an important mechanism via which a kink may reach thermal equilibrium in the pure SG chain. Although according to our estimates this would only take place on a very long time scale—beyond our present computational capacities—the fundamental importance of verifying the ergodic behavior of a prototype near-integrable system should not be underestimated.[18]

The quantitative aspects of such discretization effects yield a more favorable prospect for the practical success of continuum theory. Kink diffusion due to elastic scattering processes dominates the short time scale of the dynamics, whereas discretization effects become observable only at relatively long time scales. A dissipative Brownian motion, during the course of which a kink loses memory of its initial velocity, is estimated to occur at a time scale three orders of magnitude longer than the typical phonon or breather oscillations. Thus an experiment which determines the dynamical structure factor with a finite frequency resolution should only detect, at the high-frequency tail, the nondissipative random walk predicted by continuum theory.

APPENDIX

Using the compact notation $k=(\alpha,\theta)$ we may rewrite the quintuple integral in (13) as

$$I(\alpha)=\int d\theta\, dk'\, dk''\, \bar{\rho}(\alpha,\theta)E(k') \times E(k'')\bar{B}(k',k)\bar{B}(k'',k)\ . \tag{A1}$$

Due to the Lorentz invariance of the SG equation we have (cf. I)

$$E(k)\Delta(k,k')=E(k')\Delta(k',k) \tag{A2}$$

and

$$\int dk'\, E(k')B(k',k)=E(k)\frac{R(k)}{R_0(k)}\ , \tag{A3}$$

where $R_0(k)$ is the bare density of states, i.e., the one available to a single breather in the absence of any others. Inserting (A3) in (A1) allows us to perform the integrations over k' and k''. The result is

$$I(\alpha)=\int_0^{\pi/2} d\theta\, \bar{\rho}(\alpha,\theta)E^2(\alpha,\theta)\left[\frac{\bar{R}(\alpha,\theta)}{R_0(\alpha,\theta)}\right]^2 . \tag{A4}$$

Introducing the occupation number $n(\alpha,\theta)$ and recognizing that

$$\rho(\alpha,\theta)=R(\alpha,\theta)n(\alpha,\theta)$$

we further obtain

$$I(\alpha)=\int_0^{\pi/2} d\theta\, \bar{n}(\alpha,\theta)R_0(\alpha,\theta)E^2(\alpha,\theta)\left[\frac{\bar{R}(\alpha,\theta)}{R_0(\alpha,\theta)}\right]^3 . \tag{A5}$$

In the case of the SG breather gas

$$R_0(\alpha,\theta)=\frac{2L}{\pi d}\left[\frac{E_0}{\hbar\omega_0}\right]^2 \sin\theta\cosh\alpha\ , \tag{A6}$$

and the occupation number[7] and density of states[8] are given by

$$\bar{n}(\alpha,\theta)=\frac{(\frac{1}{2}\beta\hbar\omega_0\cosh\alpha)^2}{\sinh^2[\frac{1}{2}\beta E(\alpha,\theta)]} \tag{A7}$$

and

$$\frac{\bar{R}(\alpha,\theta)}{R_0(\alpha,\theta)}=\coth[\tfrac{1}{2}\beta E(\alpha,\theta)]-\frac{2}{\beta E(\theta,\alpha)}\ , \tag{A8}$$

respectively.

Inserting (A6)–(A8) in (A5) and defining

$$x=\beta E/2=\beta E_0\sin\theta\cosh\alpha$$

gives us in the classical, low-temperature regime $\hbar\omega_0 \ll k_B T \ll E_0$

$$I(\alpha)=\frac{2L}{2\pi}\bar{T}^2\cos\alpha\int_0^\infty dx\frac{(x\coth x-1)^3}{\sinh^2 x} =\frac{L}{2\pi d}\bar{T}^2\cosh\alpha\ . \tag{A9}$$

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[18]A very recent proposal by F. Marchesoni and C. R. Willis [Phys. Rev. A **36**, 4559 (1987)] apparently contradicts this statement by a direct perturbational calculation of higher order inelastic processes which survive the continuum limit. We will express our detailed views in a separate comment, but would like to point out that the thermalization time predicted by Marchesoni and Willis—although certainly long and in this sense not directly accessible to experiment, cf. in our discussion in Sec. IV and in the final paragraph—does fall within the range of our simulation [$\gamma_1=0.089$ for $T=0.15$ according to Eq. (26) of Marchesoni and Willis] and should have resulted in thermalization of our kink in Fig. 2.