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Dynamics of the Sine-Gordon Chain

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Using a molecular-dynamics technique, we studied some nonequilibrium properties of the sine-Gordon chain in one space dimension. We found a $t^{4/3}$ long-time tail in the mean-square displacement, and self-diffusion is traced back to the motion of kink solitons. It is shown that the propagation of these kinks gives rise to a new excitation branch.

The recent interest in solitons—especially in connection with statistical mechanics and condensed-matter physics[1-3]—makes it desirable to study the classical nonequilibrium properties of systems evolving according to such a prominent equation as the ubiquitous sine-Gordon equation. The purpose of this Letter is to report molecular-dynamics results of a classical sine-Gordon chain in one space dimension. Under the mechanical analogy, the system is defined by the Hamiltonian

$$\mathcal{H}=\sum_{i=1}^{N}\left(\frac{M\dot{X}_i^2}{2}+A(1-\cos q_0 X_i)+\frac{C}{2}(X_i-X_{i+1})^2\right). \tag{1}$$

Here i labels the particles which have mass M, while $M\dot{X}_i$ and X_i denote the corresponding momenta and displacements. M, A, C, and q_0 are parameters. We assume periodic boundary conditions so that $X_{N+1}=X_1$. In the continuum limit, Eq. (1) reduces to the sine-Gordon Hamiltonian

$$\mathcal{H}=\int H\,dX, \tag{2}$$

$$H=\frac{M\dot{f}^2}{2}+A(1-\cos q_0 f)+\frac{Ca^2}{2}\left(\frac{\partial f}{\partial x}\right)^2, \tag{3}$$

where f denotes the displacement field.

The ubiquitous role of the sine-Gordon system in condensed-matter physics derives from the variety of physical situations appearing with a periodic local potential. Examples now include one-dimensional ferromagnets with planar anisotropy,[4,5] pinned charge-density waves,[6] incommensurate phases,[7] and superionic conductors.[8] To study the relevant statistical equilibrium properties one might use the transfer-integral technique.[9] For nonequilibrium properties such as time-dependent correlation functions and spectral densities, however, we are not aware of any method providing exact results. Such correlation functions are (a) the time-dependent mean-square displacement,

$$\langle[X_i(t)-X_i(0)]^2\rangle, \tag{4}$$

and (b) the wave-number- and time-dependent density correlation function,

$$S_{\rho\rho}(q,t)=\left\langle\frac{1}{\sqrt{N}}\sum_i \exp[iqX_i(t)]\,\frac{1}{\sqrt{N}}\sum_i \exp[-iqX_i(0)]\right\rangle, \tag{5}$$

where $\langle\ \rangle$ denotes a canonical ensemble average.

To study such correlation functions, we used a molecular-dynamics technique simulating a canonical ensemble. In doing so, we assume that the particles suffer collisions with much lighter ones, representing the heat bath. The collisions are denoted by a friction $-\Gamma M\dot{X}_i$ and a random force with properties

$$\langle \eta_i(t)\rangle = 0, \qquad \langle \eta_i(t)\eta_j(t')\rangle = 2M\Gamma k_B T\delta_{ij}\delta(t-t'), \tag{6}$$

T denoting the temperature of the bath. The associated equations of motion are then coupled Langevin equations

$$M\ddot{X}_i = -\partial\mathcal{H}/\partial X_i - \Gamma M\dot{X}_i + \eta_i(t). \tag{7}$$

The stationary solution of the associated Fokker-Planck equation is the canonical distribution function.

It is clear that the nonequilibrium properties will be affected by the damping term and the random force in Eq. (7). In particular, the energy is not conserved because the Hamiltonian system is in contact with the heat bath. Nevertheless, by an appropriate choice of Γ and the chain length, τ_{ch}, over which the evolution of the system is followed, energy can be almost conserved. This choice requires

$$\tau_{ch} \gg C_T/k_B\Gamma \gg \tau_c, \tag{8}$$

where τ_c is a characteristic time of the dynamics and C_T the isothermal specific heat. The right-hand inequality also guarantees that the motions of interest do not become overdamped because of the friction term. For a more detailed description of the algorithm and the random-force generation, we refer to Schneider and Stoll.[10]

Using this molecular-dynamics technique we considered a system of 1000 particles subjected to periodic boundary conditions. The model parameters of Hamiltonian (1) were chosen as

$$M=1,\quad A=1,\quad C=29.22, \qquad q_0=\frac{2\pi}{a},\quad a=2\pi,\quad k_BT=20.86,\ 12.5,\ 8.92. \tag{9}$$

Here, we have adopted the same units as in earlier work.[11] This choice describes $CsNiF_3$ (Ref. 5) and results in a regime where solitons are expected to be important. This regime is defined by[6]

$$C \gg A,\quad E_0 = 8(AC)^{1/2} = 43.24 \gg k_BT, \tag{10}$$

where E_0 is the rest energy of the sine-Gordon kink in the continuum limit.[1]

Before discussing the numerical results, it is helpful to summarize those features of the dynamic properties that might be expected on general grounds. We expect phononlike small-amplitude and solitonlike large-amplitude motions. The frequency $\omega_A(q)$ of the phonon branch is expected to be given by[10]

$$\frac{\langle \ddot{X}(-q)\ddot{X}(q)\rangle}{\langle \dot{X}(-q)\dot{X}(q)\rangle} = M\omega_A^2 = A\langle \cos X_l\rangle + 2C(1-\cos qa), \tag{11}$$

where

$$X(q) = N^{-1/2}\sum_l X_l e^{iqal}. \tag{12}$$

At small wave vectors and much lower frequencies where we enter the *hydrodynamic* regime, we also expect the conservation laws and the large-amplitude motions to become important. Another interesting feature is the fact the the variable $X(q)$ [Eq. (12)], which is not conserved, has static correlations of infinite range, i.e., that

$$\langle |X(q)|^2\rangle = \alpha/2(1-\cos qa) \sim \alpha/(qa)^2 \text{ as } q\to 0, \tag{13}$$

as may be derived with the aid of the transfer-integral technique.[9] α depends on the model parameters and on temperature and vanishes at $T=0$. Equation (13) implies that

$$(1/N)\textstyle\sum_q \langle |X(q)|^2\rangle = \langle X_l^2\rangle = \infty. \tag{14}$$

Accordingly, the particles are not localized and *self-diffusion* will take place for $T\neq 0$. However, the implications of the conservation laws are not obvious because linearized hydrodynamics does not exist at or below two space dimensions because of long-time tails of time correlation functions.[12]

To explore the long-time tails, we calculated the time dependence of the mean-square displacement [Eq. (4)]. The second time derivative is related to the velocity autocorrelation function by

$$\frac{d^2}{dt^2}\langle [X_i(t)-X_i(0)]^2\rangle = 2\langle \dot{X}_i(t)\dot{X}_i(0)\rangle. \tag{15}$$

The results are shown in Fig. 1. For comparison we include the power law $t^{4/3}$ which was obtained for Burger's equation,[13] and mode-mode coupling considerations[12] in a one-dimensional fluid. Our data are consistent with this power law. We also note that a $t^{3/2}$ law leads to a less satisfactory agreement. This result implies that

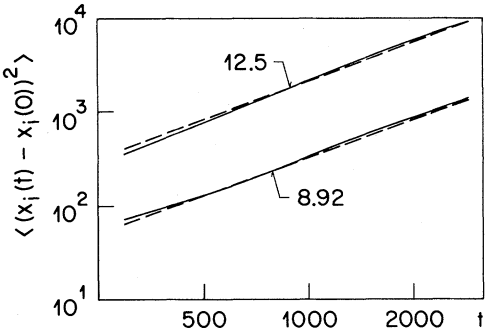

FIG. 1. Calculated time dependence of the mean-square displacement at $k_B T = 8.92$ and 12.5 for $\Gamma = 0.004$; solid lines denote numerical results and dashed lines denote $\sim t^{4/3}$ power law.

the self-diffusion coefficient does not exist. Including the temperature dependence we find consistency with the relation

$$\langle [X_i(t) - X_i(0)]^2 \rangle \sim t^{4/3} (k_B T/E_0) \exp(-E_0/k_B T) \quad (16)$$

revealing that in the regime considered here [Eq. (10)], self-diffusion is governed by moving kinks and antikinks. To explore the relevance of energy conservation on the long-time tail, we also performed a calculation for $\Gamma = 4$. The results for $\langle [X_i(t) - X_i(0)]^2 \rangle$ are again consistent with the $t^{4/3}$ power law, which indicates that the presence, or absence, of energy conservation does not affect the long-time tail.

To analyze the excitation spectrum, we calculated

$$\hat{S}_{\rho\rho}(q, \omega) = \int_{-\infty}^{+\infty} S_{\rho\rho}(q, t) e^{i\omega t} dt / S_{\rho\rho}(q, 0). \quad (17)$$

The density correlation function $S_{\rho\rho}(q,t)$ is defined in Eq. (5). The results, shown in Fig. 2, reveal that the spectral density is dominated by a low-frequency excitation branch having for $qa/\pi \geq 0.002$ a linear dispersion,

$$\omega_k = C_k q. \quad (18)$$

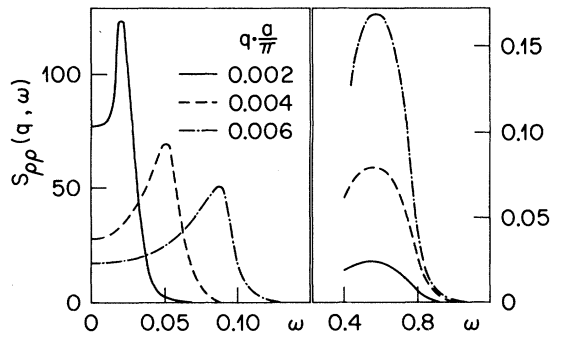

FIG. 2. $\hat{S}_{\rho\rho}(q,\omega)$ at $k_B T = 12.5$ for $\Gamma = 0.004$ and fixed reduced wave numbers qa/π, where $a = 2\pi$.

At higher frequencies, there is an additional weak resonance which we attribute to small-amplitude phononlike motions, because the peak position is consistent with Eq. (11), where $\langle \cos X_i \rangle = 0.35$ at $k_B T = 12.5$. Bearing in mind that self-diffusion has been traced back to the motion of sine-Gordon kinks, one might expect that these large-amplitude motions are also responsible for the low-frequency excitation branch in Fig. 2. To substantiate this conjecture, we also calculated the time evolution of kink patterns. For this purpose, the particles passing a maximum of the local potential [Eq. (1)] have been marked with dots. Any such passage corresponds to a kink or antikink. In Fig. 3, we show the time evolution of the resulting kink patterns for $k_B T = 12.5$. This plot demonstrates the occurrence of kinks and antikinks. Another important feature is that they propagate with a finite lifetime and a velocity C_k, where C_k is distributed around $C_k^0 \approx \pm 4a$. This value agrees with the group velocity of the low-frequnecy excitation branch ($4a$, Fig. 2). From these results, one is naturally led to the conclusion that the new, low-frequency excitation branch in Fig. 2 is due to propagating kinks and antikinks. The double-peak structure of the velocity distribution function may be qualitatively understood in terms of a relativistic Boltzmann gas.[14] The light velocity corresponds here to $C_0^2 = Ca^2$ and the mass to the kink rest mass. On this basis, it becomes clear that the new excitation branch is associated with the conservation law re-

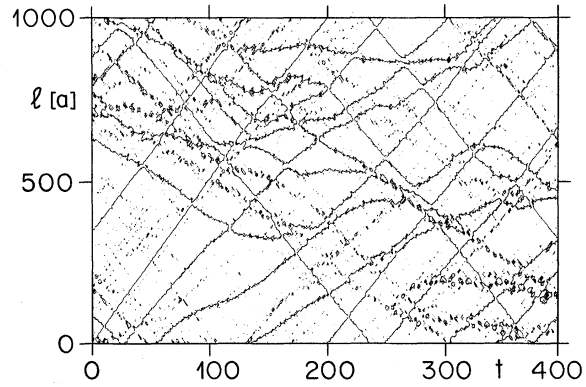

FIG. 3. Time evolution of kink patterns at $k_B T = 12.5$; l labels the particles and t denotes time. Black dots mark particles passing a maximum of the local potential. Any such passage corresponds to a kink or antikink.

sulting from the Lorentz invariance of Hamiltonian (2). The relevant conserved variable is

$$G(X,t) = tM\dot{f}\,\partial f/\partial X + (M/C_0^2)XH. \tag{19}$$

Provided that the resulting hydrodynamic mode is propagating and well defined, its frequency can be estimated to be

$$\omega_k^2 = \langle|\partial\dot{G}(q,0)/\partial q|^2\rangle/\langle|\partial H(q,0)/\partial q|^2\rangle C_0^4 \approx (qa/\pi)^4\langle|X(q)|^2\rangle\pi^4C^2(1/k_BT), \tag{20}$$

leading to $\omega_k \approx 0.030$ for $k_BT \approx 12.5$ and $qa/\pi = 1/500$, where $\langle|X(q)|^2\rangle = 8.5\times10^3$. This estimate agrees with the corresponding low-frequency peak position in Fig. 2.

To summarize, we have shown that the nonequilibrium properties of the one-dimensional sine-Gordon chain are rather rich. Our results for the mean-square displacement revealed a $t^{4/3}$ long-time tail. Moreover, at low temperatures and strong coupling [Eq. (10)], the self-diffusion was traced back to the motion of sine-Gordon kinks and antikinks. In this regime, we also found a new excitation branch due to propagating kinks. Our results also substantiate the interpretation of the low-frequency structure observed in the inelastic neutron-scattering spectrum of the one-dimensional ferromagnet $CsNiF_3$, as the result of sine-Gordon kinks.[5] However, high-resolution measurements would be needed to resolve the propagating nature of the kinks implied by our results.

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