Nondissipative diffusion of lattice solitons out of thermal equilibrium

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We perform Langevin dynamics simulations for pulse solitons on atomic chains with anharmonic nearest-neighbor interactions. After switching off noise and damping after a sufficiently long time, the solitons are only influenced by the thermal phonon bath which had been created by the noise. The soliton diffusion constant D is considerably smaller than before the switch-off, and it is proportional to the square of the temperature T, in contrast to the diffusion due to the noise which is proportional to T. We derive a diffusion equation for a soliton which is scattered elastically in an ensemble of phonons and derive general expressions for D and for the drift velocity v_d. These expressions can be evaluated for the case of the Toda lattice for which the soliton shift due to the phonon scattering is known explicitly. D is indeed proportional to T^2 and agrees well with the simulation results, while v_d is much smaller than the soliton velocity and cannot be measured in the simulations due to the large fluctuations of the soliton position. We express D in terms of soliton characteristics which are known also for solitons on other anharmonic chains in the continuum limit: namely, velocity, amplitude, and width. The results agree well with the simulations if the soliton shape is the same as in the Toda case. If the shape is different, only an estimate of the order of magnitude can be given.

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I. INTRODUCTION

We consider a family of soliton bearing lattice models: monatomic chains with anharmonic nearest-neighbor interactions. Besides the linear excitations (acoustic phonons) there are nonlinear coherent excitations: namely, solitary waves (in short solitons) which are supersonic compressional pulses. The spectrum of these nontopological excitations does not exhibit an energy gap. As a consequence the equilibrium statistical mechanics of these models (below) is very different from that of systems which bear topological solitons, like the nonlinear Klein-Gordon family.

Very recently such qualitative differences were also found when the diffusion of solitons is considered: Both pulse solitons on anharmonic chains [1] and pulse solitons on classical isotropic Heisenberg spin chains [2] exhibit a *superdiffusive* behavior: The variance $\sigma^2(t)$ of the soliton position $X(t)$ contains anomalous terms proportional to t^2 or t^3, in addition to the normal random walk term Dt, where D is the soliton diffusion constant and t is the time. These superdiffusive terms were obtained by collective variable (CV) theories which include, besides the soliton position, additional variables like the width or amplitude of the soliton. The normal linear term in σ^2 stems from the soliton shifts due to the "kicks" of the white noise which models the thermal fluctuations. In contrast to this direct effect, the superdiffusive terms represent an *indirect* effect which stems from distortions of the soliton shape (due to the noise) which in turn change the soliton velocity and thus in the end the soliton position.

The above predictions of the CV theory for the lattice solitons were confirmed by Langevin-dynamics (LD) simulations [1]. However, there is one exception: For low-energy solitons (with velocities very close to the sound velocity) the observed variance σ^2_{LD} is larger than predicted (but linear in t; the superdiffusive contributions are negligible in this velocity regime). The difference between σ^2_{LD} and the result σ^2_{CV} from CV theory was explained by the influence of the phonons which are not taken into account in the CV theory: After switching off noise and damping in the LD simulations after a sufficiently long time t_s, the solitons are only influenced by the phonon bath which has been created by the noise. For $t>t_s$ the simulations are molecular-dynamics (MD) simulations. Here the solitons show a normal diffusion $\sigma^2_{MD}=D_{MD}t$. The difference $D_{LD}-D_{MD}$ in the slopes before and after the switch-off agrees very well with D_{CV}. This result clearly confirms the collective variable theory, and it strongly suggests that D_{MD} is equal to the diffusion constant D_{ph} of a soliton in a thermal phonon bath.

The aim of our paper is to calculate D_{ph} and to compare with D_{MD} from simulations. It is important to note that D_{ph} is not related to a viscosity, via an Einstein relation, because in our random walk problem *no dissipation* is involved for two reasons: (i) We consider a Hamiltonian system (no noise and damping), and (ii) the solitons are scattered elastically by the phonons, because our solitary waves are exact solutions which are stable against perturbations by linear excitations (phonons). The nonintegrability of our systems would only be important if we consider soliton-soliton scattering where the solitons loose energy due to radiation of phonons.

For the kink solitons of the sine-Gordon model, $D_{ph}\sim T^2$, where T is the temperature of the phonon bath, was predicted already a long time ago [3–6]. We will use essentially the same methods; however, compared to this model, some important differences will show up in Sec. III. Moreover, the MD simulations are different, too: The sine-Gordon system must be discretized which produces an artifact: namely, a Brillouin zone for the phonon states. The unwanted effects due to this artifact can only partially be avoided by certain tricks—e.g., Ref. 6. Such tricks are not necessary for our lattice model which is discrete anyway.

We will proceed in the following way.

(a) We first consider the Toda lattice [7], because it is the only lattice model for which the soliton shift due to scattering with phonons was calculated exactly [8].

(b) Our result for D_{ph} can be written as a function of soliton characteristics: namely, the soliton velocity, amplitude, and width. Therefore our result can be generalized to other anharmonic chains for which these characteristics are known.

(c) The results of (a) and (b) are tested by MD simulations for the Toda lattice and for the case of interaction potentials with cubic and quartic anharmonicities.

Finally we would like to stress that we consider a *nonequilibrium* situation: a single soliton with a given velocity in a thermal bath of phonons. In contrast to this, the diffusion of an ensemble of solitons in thermal *equilibrium* was recently investigated for the case of the Toda lattice [9] by using earlier results from Bethe ansatz theory for the Toda lattice [10].

However, in contrast to topological solitons (e.g., sine-Gordon kinks), the nontopological Toda solitons do *not* yield a clear-cut evidence of their existence in thermal equilibrium. This holds both for static properties, like the specific heat, and for dynamical quantities, like the dynamic form factor (Fourier transform of the displacement autocorrelation); see the brief summary in the Appendix. For this reason the soliton diffusion constant in Ref. [9] is in fact an intermediate result which cannot be tested by MD simulations. It appears, however, as an input for the kinetic energy autocorrelation, which was confirmed by the simulations.

It is possible in principle that a mode-mode coupling approach could reproduce some of the effects we find and confirm them by direct numerical simulations for the low-amplitude excitations we consider. However, such approaches lose the information of solitonlike coherence, which we find to persist to long times. This is important for the extension of our Toda lattice results to more general nonlinear lattice potentials. The particlelike coherence and its response to the environment of phonons in the same nonlinear lattice are an explicit example of optimal coarse graining in a complex system and therefore to intelligent multiscale modeling. The particlelike excitation represents an important scale for physical properties, and it interacts with a bath of modes provided self-consistently by the same lattice without interaction with an *ad hoc* external environment.

II. TRANSPORT EQUATION FOR SOLITON DIFFUSION

We use standard procedures to derive a diffusion equation for a soliton which is scattered elastically in an ensemble of phonons. We mostly follow Refs. [4,5] in which the diffusion of kink solitons in the sine-Gordon model was considered. However, compared to this model some important differences will show up, both for the analytical calculations and for the MD simulations.

We consider a time interval τ in which a soliton with velocity v collides with n_q phonons of wave number q and suffers spatial shifts $\Delta_q(v)$. The collision time is assumed to be much smaller than τ. The total shift of the soliton during τ is

$$\Delta_{\rm tot}(v) = \sum_q n_q \Delta_q(v). \tag{1}$$

For the probability $P(x,t)dx$ to find the soliton at time t in the interval $(x, x+dx)$ we have the master equation

$$P(x,t+\tau) = P(x - v\tau, t) + \sum_{\{n_q\}} P(x - v\tau - \Delta_{\rm tot}, t) W(\{n_q\},\tau) - \sum_{\{n_q\}} P(x - v\tau, t) W(\{n_q\},\tau). \tag{2}$$

Here $W(\{n_q\},\tau)$ is the probability that $\{n_q\}=n_{q_1}, n_{q_2}, \ldots$ phonons collide during τ. A Taylor expansion up to first order in τ yields

$$\tau\frac{\partial P}{\partial t} = - v\tau\frac{\partial P}{\partial x} - \frac{\partial P}{\partial x}\sum_{\{n_q\}} W\Delta_{\rm tot} + \frac{1}{2}\frac{\partial^2 P}{\partial x^2}\sum_{\{n_q\}} W(-2v\tau\Delta_{\rm tot} + \Delta_{\rm tot}^2). \tag{3}$$

Dividing by τ and using Eq. (1) we obtain the diffusion equation

$$\frac{\partial P}{\partial t} = -(v + v_d)\frac{\partial P}{\partial x} + D_{ph}\frac{\partial^2 P}{\partial x^2}, \tag{4}$$

with the drift velocity

$$v_d = \frac{1}{\tau}\sum_{\{n_q\}} W(\{n_q\},\tau)\sum_q n_q\Delta_q \tag{5}$$

and the soliton diffusion constant

$$D_{ph} = \frac{1}{2\tau}\sum_{\{n_q\}} W(\{n_q\},\tau)\sum_{q,q'} n_q n_{q'}\Delta_q\Delta_{q'}. \tag{6}$$

We remark that the third term on the right-hand side (RHS) of Eq. (3) yields a contribution to D_{ph} that is proportional to $vv_d\tau$, which has to be omitted in order to get a consistent expansion in τ.

We now assume the independence of the collisions with phonons of different wave numbers which means that W factorizes

$$W(\{n_q\},\tau) = \prod_j w(n_{q_j},\tau). \tag{7}$$

We then obtain

$$v_d = \frac{1}{\tau}\sum_q \Delta_q\langle n_q(\tau)\rangle, \tag{8}$$

where

$$\langle n_q(\tau)\rangle = \sum_{n_q} n_q w(n_q,\tau) \tag{9}$$

is the average number of phonons which collide with the soliton during τ. The double sum in Eq. (6) can be split into off-diagonal and diagonal parts:

$$D_{ph} = \frac{1}{2\tau}\left\{ \sum_{q \neq q'} \Delta_q \Delta_{q'} \langle n_q \rangle \langle n_{q'} \rangle + \sum_q \Delta_q^2 \langle n_q^2 \rangle \right\}. \tag{10}$$

Adding the term with $q=q'$ to the first sum and subtracting it from the second sum we obtain

$$D_{ph} = \frac{1}{2} v_d^2 \tau + \frac{1}{2\tau} \sum_q \Delta_q^2 \{ \langle n_q^2 \rangle - \langle n_q \rangle^2 \}. \tag{11}$$

Here the term linear in τ has to be omitted in order to be consistent with the above neglection of other linear terms [formally one would like to take the limit $\tau \to 0$ in Eqs. (8) and (11), but on the other hand, τ must be much larger than the collision time]. The final result

$$D_{ph} = \frac{1}{2\tau} \sum_q \Delta_q^2 \mathrm{Var}[n_q(\tau)] \tag{12}$$

for the soliton diffusion constant only depends on the shifts Δ_q of the soliton and on the variance of the number of phonons which collide with the soliton.

We first evaluate the drift velocity in Eq. (8). $\langle n_q(\tau) \rangle$ is the product of the phonon current and the duration τ of the interval

$$\langle n_q(\tau) \rangle = \frac{\langle N_q \rangle}{L} |v_{rel}| \tau. \tag{13}$$

Here L is the length of the system and $\langle N_q \rangle / L$ is the phonon density—i.e., the average number of phonons of wave number q per unit length. $v_{rel}=v+v_d-v_q$ is the relative velocity between the soliton and phonons with group velocity $v_q = d\omega_q / dq$, where ω_q is the phonon dispersion curve. In v_{rel} the drift velocity v_d must be included which means that Eq. (8) yields an implicit equation for v_d:

$$v_d = \frac{1}{L} \sum_q \Delta_q \langle N_q \rangle |v + v_d - v_q|. \tag{14}$$

For D_{ph} we need $\mathrm{Var}(n_q)$. We divide L in a large number K of equal intervals of length L/K, where each interval $i=1,2,\ldots,K$ carries N_q^i phonons. We choose K such that the interval length equals the distance which the phonons with velocity v_q travel during the time τ in the soliton's rest frame—i.e., $L/K = |v_{rel}|\tau$. Then $n_q(\tau)$ is equal to N_q^i. The total phonon number N_q is the sum over all N_q^i. One can easily show that $\mathrm{Var}(N_q) = K \mathrm{Var}(N_q^i)$, assuming that the phonons in different intervals are statistically independent. We then obtain $\mathrm{Var}[n_q(\tau)] = L^{-1} \mathrm{Var}(N_q) |v_{rel}| \tau$ and finally

$$D_{ph} = \frac{1}{2L} \sum_q \Delta_q^2 \mathrm{Var}(N_q) |v + v_d - v_q|. \tag{15}$$

We treat a classical model, but it is convenient to start with the Bose-Einstein statistics for the phonons and to take the classical limit later:

$$\langle N_q \rangle = [e^{\beta(E_q - \mu)} - 1]^{-1}, \tag{16a}$$

$$\mathrm{Var}(N_q) = k_B T \frac{\partial}{\partial \mu} \langle N_q \rangle = \langle N_q \rangle (\langle N_q \rangle + 1); \tag{16b}$$

see Ref. [11], for instance. E_q and μ are the energy and chemical potential of the phonons with wave number q. Since the phonon number is not fixed, μ is zero which is inserted after the differentiation in Eq. (16).

In the classical limit each phonon state q is highly populated (formally the high-temperature limit):

$$\langle N_q \rangle = k_B T / E_q \gg 1, \tag{17a}$$

$$\mathrm{Var}(N_q) = \langle N_q \rangle^2. \tag{17b}$$

In q space the phonon density is $\langle N_q \rangle L / (2\pi)$ and its variance $\langle N_q \rangle^2 L / (2\pi)$. Thus the relative fluctuations are $\sqrt{2\pi/L}$, as expected.

With Eqs. (17), (13), (12), and (8) we finally obtain

$$v_d = k_B T \frac{1}{L} \sum_q \frac{\Delta_q}{E_q} \quad |v + v_d - v_q|, \tag{18a}$$

$$D_{ph} = \frac{1}{2} (k_B T)^2 \frac{1}{L} \sum_q \left(\frac{\Delta_q}{E_q} \right)^2 |v + v_d - v_q|. \tag{18b}$$

III. DRIFT VELOCITY AND DIFFUSION CONSTANT FOR TODA SOLITONS

The nearest-neighbor interaction potential of the Toda lattice [7] can be written as

$$\tilde{V}(\tilde{r}_n) = \frac{m\omega^2}{\gamma^2} \{ e^{-\gamma \tilde{r}_n} + \gamma \tilde{r}_n - 1 \}. \tag{19}$$

$\tilde{r}_n$ is the relative displacement of particle n, m is the mass of the particles, γ is the anharmonicity parameter, and ω is the frequency in the harmonic limit $(\gamma \to 0)$. Following most of the literature we will work with the dimensionless form

$$V(r_n) = e^{-r_n} + r_n - 1, \tag{20}$$

but we will return to the original units whenever necessary for the discussion of results. For this return we must take into account that the system has two length scales: $1/\gamma$ and the lattice constant a.

The solutions of the linearized equations of motion are acoustic phonons with

$$\omega_q = 2 \left| \sin \frac{q}{2} \right|, \quad -\pi < q \leq \pi, \tag{21a}$$

$$v_q = \pm \cos \frac{q}{2}, \tag{21b}$$

where the upper (lower) sign holds for positive (negative) q. The speed of sound is $c=1$. The one-soliton solution is

$$e^{-r_n(t)} - 1 = \sinh^2 \alpha \, \mathrm{sech}^2 [\alpha (n - v_\alpha t)], \tag{22a}$$

$$v_\alpha = \pm \frac{\sinh \alpha}{\alpha}, \tag{22b}$$

where the parameter $\alpha > 0$ determines all properties of the soliton. We will always consider a positive soliton velocity v_α—i.e., movement to the right.

Due to the scattering with the soliton, the phonons suffer phase shifts δ_q which were calculated by different methods [8,12,13]:

$$\tan(\delta_q/4) = \begin{cases} \coth(\alpha/2)\tan(q/4), & 0 \leqslant q \leqslant \pi, \\ \tanh(\alpha/2)\tan(q/4), & -\pi < q \leqslant 0. \end{cases} \tag{23}$$

The change of the phonon density of states due to the presence of the soliton is

$$\Delta\varrho(q) = -\frac{1}{2\pi}\frac{d\delta_q}{dq}, \tag{24}$$

and the total number of phonon states is reduced by 1:

$$\int_{-\pi}^{\pi} d_q \Delta\varrho(q) = -1. \tag{25}$$

Considering a lattice with finite length L one can see [8] that the removed state is the standing wave at the right edge $q=\pi$ of the Brillouin zone. The states around $q=0$ are not changed (in first order in $1/L$), and the state $q=0$ is not changed at all; this is a consequence of translational invariance which is not destroyed by a Toda soliton because it is a pulse soliton. By contrast, in the presence of topological solitons, like the sine-Gordon kinks, the $q=0$ state is removed (if the kink is static; if it is moving, the state with the same group velocity is removed).

For the above reasons the density of states is changed only near the edge of the Brillouin zone, where the phonon energies show a maximum. These phonons are not much excited for low temperatures, which means that we can use the unchanged density of states when we replace the sums in Eqs. (18) by integrals:

$$\frac{1}{L}\sum_q \cdots = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \cdots . \tag{26}$$

The most important ingredient for the explicit calculation of v_d and D_{ph} is the soliton shift Δ_q. In contrast to δ_q which was calculated by considering a plane-wave phonon [8,12] or by performing a linear-stability analysis [13], a phonon wave packet had to be considered [8] in order to get Δ_q. The wave packet is defined by a distribution function $R(k)$ in k space, peaked around q, with an amplitude A and a width $\Gamma \ll |q|$. The result of Ref. [8] is

$$\Delta_q = \mp \frac{A^2}{2\Gamma}\frac{v_\alpha}{\cosh\alpha \mp \cos q/2}, \tag{27}$$

where the upper signs hold for head-tail collisions ($q>0$) and the lower ones for head-on collisions ($q<0$). However, Eq. (27) does not hold for $q\to 0$ because the condition $\Gamma \ll |q|$ can no longer be fulfilled. In fact, Eq. (27) yields an unphysical result for $q \to 0$: As the energy of the wave packet is

$$E_q = \frac{1}{2}\frac{A^2}{\Gamma}\omega_q^2, \tag{28}$$

we get, for the quotient Δ_q/E_q appearing in v_d and D_{ph},

$$\frac{\Delta_q}{E_q} = \mp \frac{1}{\omega_q^2}\frac{v_\alpha}{\cosh\alpha \mp \cos q/2}, \tag{29}$$

which diverges for $q\to 0$. However, a simple consideration shows that Δ_q must actually vanish in this limit: Consider a soliton and a phonon with a wavelength in the order of the length L of the system. Here the soliton *sits* on a very long wave whose displacement field does not vary over the width of the soliton. Thus the soliton cannot be influenced and is not shifted at all. In order to take into account this feature we introduce a cutoff q_c; i.e., we set $\Delta_q \equiv 0$ for $q < q_c \ll 1$, but q_c must be much larger than $q_{min}=2\pi/L$. On the other hand, q_c should be smaller than the inverse soliton width α, because we expect the maximum shift Δ_q when soliton and phonon have about the same width.

We want to insert Eq. (29) into Eqs. (18) which have been derived in a semiclassical approach where $E_q=\hbar\omega_q$. However, E_q in Eq. (28) is the energy of a classical phonon wave packet defined by the distribution function $R(k)$ in k space [see above Eq. (27)]. The equivalence of the two approaches was shown by identifying the phonon action variable $J(k)$ with $\hbar R(k)$, using inverse scattering theory [8].

v_d (and also D_{ph}) consists of two contributions stemming from the head-on and head-tail collisions. Using Eqs. (18a), (26), and (29) and the cutoff we obtain

$$v_d = Tv_\alpha\left\{\int_{-\pi}^{-q_c}\frac{dq}{2\pi\omega_q^2}\frac{v_\alpha + \cos q/2}{\cosh\alpha + \cos q/2} - \int_{q_c}^{\pi}\frac{dq}{2\pi\omega_q^2}\frac{v_\alpha - \cos q/2}{\cosh\alpha - \cos q/2}\right\}. \tag{30}$$

Here we have neglected v_d on the rhs of Eq. (18a), because an iterative solution of Eq. (18a), starting with $v_d^{(0)}=0$, shows that $v_d^{(1)}=O(T)$. Thus the next contribution is of $O(T^2)$ which can be neglected for low temperatures (K_BT much smaller than the soliton energy).

Equation (30) yields

$$v_d = Tv_\alpha(\cosh\alpha - v_\alpha)\int_{q_c}^{\pi}\frac{dq}{2\pi\omega_q^2}\frac{2\cos q/2}{\cosh^2\alpha - \cos^2 q/2},$$

$$= \frac{Tv_\alpha(\cosh\alpha - v_\alpha)}{2\pi\sinh^2\alpha} \times\left\{\frac{1}{\sin q_c/2} + \frac{1}{\sinh\alpha}\left(\arctan\frac{\sin q_c/2}{\sinh\alpha} - \arctan\frac{1}{\sinh\alpha}\right) - 1\right\}. \tag{31}$$

Using $q_c \ll 1$ the result simplifies to

$$v_d = \frac{T v_\alpha(\cosh\alpha - v_\alpha)}{2\pi \sinh^2\alpha}\left\{\frac{2}{q_c} - \frac{1}{\sinh\alpha}\left(\frac{\pi}{2} - \arctan(\sinh\alpha) - \arctan\frac{q_c/2}{\sinh\alpha}\right)\right\}. \tag{32}$$

The soliton diffusion constant D_{ph} in Eq. (18b) can be calculated in the same way as v_d, but here the contributions from head-on and head-tail collisions add up, whereas they nearly compensated each other in v_d:

$$D_{ph} = \frac{1}{2}T^2 v_\alpha^2 \int_{q_c}^{\pi} \frac{dq}{2\pi\omega_q^4}\left\{\frac{v_\alpha + v_d + \cos q/2}{(\cosh\alpha + \cos q/2)^2} + \frac{v_\alpha + v_d - \cos q/2}{(\cosh\alpha - \cos q/2)^2}\right\}. \tag{33}$$

Since $v_d = O(T)$, it contributes a term of $O(T^3)$ to D_{ph} which can be neglected for low temperatures. The evaluation of the integral in Eq. (33) yields a very long expression which simplifies considerably for $q_c \ll 1$:

$$D_{ph} = \frac{T^2 v_\alpha^2}{4\pi \sinh^4\alpha}\left\{\frac{1}{3}\frac{v_\alpha(3+\cosh 2\alpha) - 4\cosh\alpha}{q_c^3} - \frac{\pi}{8}\frac{3 - 5v_\alpha\cosh\alpha + 2\cosh 2\alpha}{\sinh^3\alpha}\right\}. \tag{34}$$

Let us first discuss the drift velocity v_d. The integrals (30) contain the expression

$$\frac{v_\alpha \pm \cos q/2}{\cosh\alpha \pm \cos q/2} = \frac{v_\alpha - v_q}{V_\alpha - v_q}, \tag{35}$$

where

$$V_\alpha = E_\alpha / P_\alpha \tag{36}$$

is a *new characteristic velocity* which controls the soliton-phonon scattering together with the soliton velocity $v_\alpha = P_\alpha / M_\alpha$ and the phonon group velocity v_q. $P_\alpha = \sinh 2\alpha$ is the (kinetic) momentum of the soliton, which is different from its canonical momentum $P_\alpha^{can} = 4(\alpha\cosh\alpha - \sinh\alpha)$ [14,15]. $M_\alpha = 2\alpha$ is the soliton mass (excess mass due to the compression of the lattice [7]). $E_\alpha = \sinh 2\alpha$ is the soliton energy, when the linear term in the potential (20) is omitted [7]. This term only influences the energies, not the dynamics; moreover, it drops out for periodic boundary conditions which are used in our MD simulations. The above interpretation of V_α is supported by the final result (32) which shows that

$$v_d \sim V_\alpha - v_\alpha; \tag{37}$$

i.e., the drift velocity is nonzero only because V_α is different from v_α.

Interestingly, the difference (37) has some similarity with the difference between the phase and group velocities of the phonons:

$$V_q - v_q = \frac{\omega_q}{q} - \frac{d\omega_q}{dq} = \frac{E_q}{P_q} - \frac{dE_q}{dP_q}, \tag{38}$$

with $E_q = \hbar\omega_q$ and $P_q = \hbar q$ in semiclassical language. This similarity is increased by noting that the soliton velocity $v_\alpha = \dot{Q}_\alpha$ appears in the Hamilton equation $\dot{Q}_\alpha = \partial E_\alpha^{can} / \partial P_\alpha^{can}$, where Q_α is the soliton position. $E_\alpha^{can} = E_\alpha - 2\alpha$ is the soliton energy when the compression energy 2α is included. Since E_α^{can} does not depend on Q_α, we can finally write

$$V_\alpha - v_\alpha = \frac{E_\alpha}{P_\alpha} - \frac{dE_\alpha^{can}}{dP_\alpha^{can}}. \tag{39}$$

Now the analogy with Eq. (38) is perfect because for the phonons there is no difference between kinetic and canonical momenta.

Finally we want to simplify our results (32) and (34), because in our MD simulations we only consider solitons with $\alpha \ll 1$. For this case,

$$v_d = \frac{T}{3\pi}\left\{\frac{1}{q_c} - \frac{1}{2\alpha}\left(\frac{\pi}{2} - \arctan\frac{q_c}{2\alpha}\right)\right\}, \tag{40}$$

$$D_{ph} = \frac{T^2}{4\pi}\left(\frac{2}{9}\frac{1}{q_c^3\alpha^2} - \frac{\pi}{12}\frac{1}{\alpha^5}\right). \tag{41}$$

IV. LANGEVIN DYNAMICS PLUS MD SIMULATIONS FOR THE TODA LATTICE

Since we want to study a single soliton in a thermal phonon bath, we cannot start with Monte Carlo simulations where many solitons would be present which cannot be tracked (see the Appendix). Therefore we first perform Langevin-dynamics simulations; i.e., we start with a one-soliton solution, and then we numerically integrate the equation of motion for a lattice of length $L=1500$, including white-noise and damping terms [1]. After a sufficiently long time t_s, when the phonon bath is well established, both noise and damping are switched off, but the integration continues as an MD simulation up to the final time t_f. The soliton position $X(t)$ is obtained by a rather involved method [1], because the soliton shape can be very significantly masked by the fluctuations, depending on the chosen parameters (below).

The runs are repeated many times (typically 200) with different random numbers producing the white noise; i.e., in each run we have a different configuration at t_s. Finally the variance $\sigma^2(t) = \langle X^2\rangle - \langle X\rangle^2$ is computed as an average over all the runs.

The results are fitted to two straight lines for $t \leq t_s$ and $t \geq t_s$, respectively. Figure 1 shows a case where the initial soliton velocity is very close to the sound velocity (which means very low energy) and the temperature is relatively high, which results in a very noisy soliton and a large variance. For higher energy and/or lower temperature the variance is smaller.

The slopes of the straight lines are denoted by D_{LD} for $t \leq t_s$ and D_{MD} for $t \geq t_s$. D_{LD} was investigated in Ref. [1],

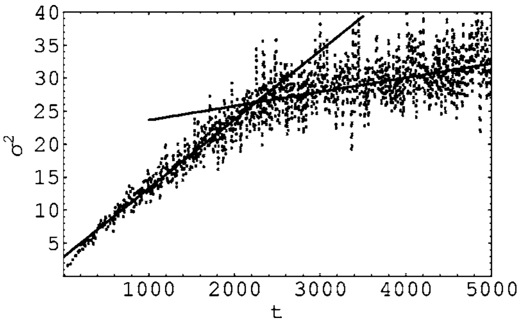

FIG. 1. Variance of soliton position vs time t for a Toda soliton with $v_\alpha=1.001$—i.e., $\alpha=0.07746$—and temperature $T=10^{-4}$. At the time $t_s=2500$ noise and damping were switched off.

while we are interested here in D_{MD} which has to be compared to D_{ph} in Eq. (41). [It was not possible to determine the drift velocity and compare with Eq. (40), because it is much smaller than v_α and the fluctuations in $X(t)$ are large.]

In order to test the main prediction of Eq. (41)—namely, $D_{ph}\sim T^2$—we fitted a quadratic function to our data of D_{MD} for different initial velocities v_α; α is determined by Eq. (22b) (Fig. 2). For all v_α the soliton energy E_α is much larger than k_BT. The fits are fairly good and thus we can now determine the cutoff wave number q_c by setting $D_{ph}(\alpha,q_c,T)=D_{MD}(\alpha,T)$. We obtain $q_c=0.031$, 0.049, and 0.039 for $\alpha=0.077\,46$, 0.1731, and 0.2446, respectively. This means that q_c in fact fulfills the conditions made below Eq. (29): It is much larger than $2\pi/L=0.0042$, and it is in fact smaller than α and roughly constant; i.e., the cutoff is made far below the maximum soliton shift around $q=\alpha$, as anticipated in Sec. III.

V. GENERALIZATION TO OTHER ANHARMONIC CHAINS

We proceed in several steps. *First*, we performed simulation in which the Toda potential (20) was replaced by an expansion up to fourth order in r_n. The results are undistinguishable from those for the Toda lattice. Thus complete integrability is not important, as anticipated already in the introduction.

Second, we express D_{ph} in Eq. (34) by soliton characteristics which are familiar also for solitons on other anharmonic chains in the continuum limit: namely, velocity, amplitude, and width. In the prefactor in D_{ph} we easily identify the velocity $v_\alpha := v$ and the amplitude $\sinh^2\alpha := A$. [Here we have assumed small displacements r_n in Eq. (22a).] The braces in Eq. (34) contain expressions which have no direct interpretation. Therefore we expand for $\alpha \ll 1$ and identify the width $\alpha^{-1} := b$ and obtain

$$D_{ph} = \frac{T^2}{4\pi}\frac{v^2 b}{A^2}\left\{\frac{2}{9(bq_c)^3} - \frac{\pi}{12}\right\}. \tag{42}$$

Third, we choose a potential with a negative cubic anharmonicity $-\frac{1}{3}r_n^3$, because then the solitons have the same shape as on the Toda lattice—namely, $r(x,t)=-A\,\mathrm{sech}^2\{(x-vt)/b\}$—but the relations between A, v, and b are different:

$$A = \frac{3}{2}(v^2-1), \quad b=[3(v^2-1)/v^2]^{-1/2}. \tag{43}$$

The MD simulations exhibit again a clear T^2 dependence (Fig. 3), but D_{MD} is much larger than for the Toda lattice [cf. Fig. 2(c) with the same velocity]. This is qualitatively explained by the factor $1/A^2$ in Eq. (42), because A is much

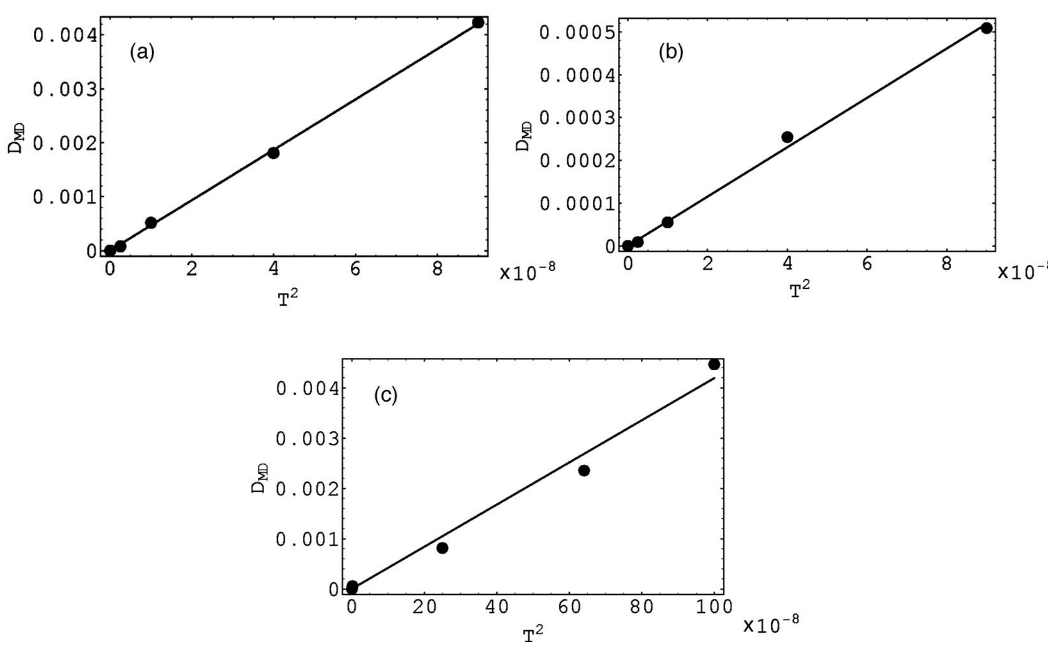

FIG. 2. Diffusion constant D_{MD} vs temperature square T^2 for Toda solitons. Circles: data from MD simulations. Solid lines: fit by $D_{MD}=CT^2$ (a) $v_\alpha=1.001$—i.e., $\alpha=0.07746$, $C=46735.0$. (b) $v_\alpha=1.005$—i.e., $\alpha=0.1731$, $C=5763.38$. (c) $v_\alpha=1.01$—i.e., $\alpha=0.2446$, $C=4193.95$.

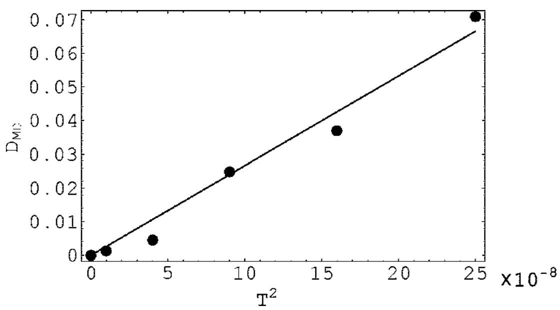

FIG. 3. Diffusion constant D_{MD} vs temperature square T^2 for a soliton with $v=1.01$ on a chain with cubic anharmonicity. Circles: data from MD simulations. Solid line: fit by CT^2 with $C=266267.0$.

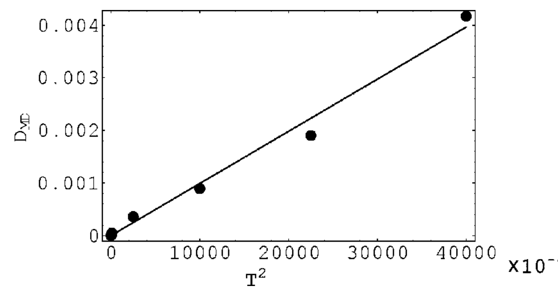

FIG. 4. Diffusion constant D_{MD} vs temperature square T^2 for a soliton with $v=1.001$ on a chain with quartic anharmonicity. Circles: MD data. Solid line: fit by CT^2 with $C=9.91581$.

smaller, but b is not changed much, compared to the Toda lattice. In the case of a positive cubic anharmonicity the solitons are rarefactive pulses, instead of compressional ones. But this does not change D_{ph}, because the soliton shift Δ_q enters quadratically in Eq. (18b), and this is confirmed by the MD simulations.

Our *fourth* and last step is to choose a potential with quartic anharmonicity $\frac{1}{4}r_n^4$. Here the solitons have the shape $r(x,t)=\pm A\ \mathrm{sech}\{(x-vt)/b\}$—i.e., rarefactive or compressional pulses—with

$$A=[2(v^2-1)]^{1/2}, \quad b=[12(v^2-1)/v^2]^{-1/2}. \tag{44}$$

However, as the sech shape differs considerably from the sech^2 shape of the Toda solitons the soliton shift Δ_q and the soliton diffusion constant D_{ph} must also differ considerably from the Toda lattice results (29) and (42), respectively. Nevertheless, the T^2 dependence of D_{ph} is not affected and this is indeed confirmed by the MD simulations (Fig. 4).

Moreover, we can estimate the order of magnitude of D_{ph}: For $v=1.001$ we have $A=0.0633$ from Eq. (44), which is more than a factor of 10 larger than the Toda soliton amplitude 0.0060. The effective soliton width, defined as the distance for which r drops by $\mathrm{sech}^2\,1=0.42$, is not much different from the Toda case. Therefore the dominant dependence in Eq. (42) is $D_{ph}\sim 1/A^2$, which means that D_{ph} should be smaller by roughly a factor of 110 compared to the Toda case. This means that the solitons on the chain with quartic anharmonicity should be much more robust than Toda solitons; i.e., they are much less affected by the scattering with phonons and thus their diffusion constant is much smaller. This is indeed confirmed by the MD simulations (Fig. 4), but only roughly because D_{MD} is smaller than our estimate by a factor of 16. Our estimate could be improved if we would know the cutoff wavelength q_c which is certainly different from the Toda case since Δ_q is different. The mechanism we propose is presumably still effective, but Δ_q is not known as for Toda-like cases; we can of course anticipate that the softer pulse shape implies a cutoff in larger q than the cubic cases.

VI. CONCLUSIONS

The effects of thermal noise on solitons have been successfully modeled here by including white noise and damping in the microscopic equations of motion. In the case of pulse solitons on anharmonic chains there are three different mechanisms which contribute to the diffusion of the solitons.

(i) The *kicks* of the noise on the atoms of the chain cause effectively a shift of the soliton position. This yields a *normal* diffusive behavior; i.e., the variance $\sigma^2(t)$ of the soliton position contains a random walk term which is proportional to the time t.

(ii) The noise also causes a change of the soliton's shape; e.g., its width and amplitude are changed. As the soliton velocity is a function of these parameters, the velocity is also changed which eventually yields a *superdiffusive* term in the variance—i.e., a term proportional to t^2. Both the normal linear term and the anomalous quadratic term were calculated in a collective variable theory and confirmed by Langevin dynamics simulations [1].

(iii) The noise also produces phonons which scatter elastically with the solitons which thus suffer spatial shifts. When the noise has acted for a sufficiently long time, a thermal phonon bath is created which produces a *nondissipative* diffusion.

Our theory for this contribution yields $D_{ph}t$, where $D_{ph}\sim T^2$, in contrast to the first two contributions which both have diffusion constants proportional to the temperature T. The phonon contribution $D_{ph}t$ to the variance $\sigma^2(t)$ can be observed best in simulations, when noise and damping have been switched off so that the first two contributions to σ^2 vanish. The predicted T^2 dependence of D_{ph} is indeed very well confirmed by our simulations for all anharmonic lattices we have investigated: chains with a Toda interaction potential, a truncated Toda potential, and potentials with cubic or quartic anharmonicities.

In the case of the Toda lattice the factor C in $D_{ph}=CT^2$ has been used to determine the cutoff wave number q_c which avoids the long-wavelength divergence in the soliton shift. It turns out that the cutoff is made far below the maximum shift around $q=\alpha$, as anticipated. For the other cases, the same q_c as in the Toda lattice has been used. In the case of the cubic anharmonicity D_{ph} agrees qualitatively with the simulations, because here the solitons have the same shape as in the Toda lattice. However, the shape is different in the case of a quartic anharmonicity; thus, the formula for the soliton shift is not valid here and an agreement cannot be expected without a separate determination of this spatial shift.

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APPENDIX: EQUILIBRIUM STATISTICAL MECHANICS OF THE TODA LATTICE

The free energy of the lattice under zero pressure can be calculated exactly [7]:

$$F = \frac{1}{\beta}\{\ln \beta - \beta + (\beta - 1/2)\ln \beta - \ln[\Gamma(\beta)/\sqrt{2\pi}]\}, \quad \text{(A1)}$$

where Γ is the gamma function and $\beta = 1/T$. A low-temperature expansion yields

$$F = -T \ln T - T^2/12 + \cdots , \quad \text{(A2)}$$

where the first term is identical with the free energy of a harmonic lattice and thus the second term is an anharmonic contribution, which in fact can also be obtained as the leading term in an anharmonic perturbation theory.

In contrast to this, the corresponding term in the free energy of systems which bear topological solitons, like the sine-Gordon model, cannot be obtained by a perturbation theory. The reason is that this term is proportional to $\exp(-\beta E_s)$, where E_s is the soliton energy, and thus has an essential singularity at $T=0$. However, this term can be identified with the free energy F_s of a soliton gas [16].

For the Toda lattice such a soliton gas identification was tried, but was not possible. Here $F_s \sim T^{4/3}$, where the phonon phase shifts were taken into account [17]. Including the soliton phase shifts, this term is canceled; the T^2 term in Eq. (A2) turns out to stem from phonon-phonon scattering [18,19]. Thus there is no soliton signature in the free energy, specific heat, and other static quantities of the Toda lattice.

For dynamic quantities the situation is quite similar. The dynamic form factor $S(q,\omega)$, the Fourier transform of the displacement-displacement correlation function, exhibits two neighboring peaks in a phonon plus soliton gas phenomenology if all phase shifts are neglected [20]. However, this two-peak structure was not confirmed by combined Monte Carlo (MC) and MD simulations [21] which show only one peak. This peak exhibits Lorentzian and exponential tails on the low- and high-frequency sides, respectively, as predicted by the phonon and soliton gas approaches.

Interestingly, small soliton peaks could be identified on the high-frequency shoulder if the MD simulations were started with initial conditions stemming from certain *non-equilibrium* configurations taken from incomplete MC runs [22]. This means that only solitons with a relatively high energy, and out of thermal equilibrium, can be identified. The same holds when one tries to observe solitons directly by tracking them in the displacement pattern of the MD simulations.

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