Envelope solitons on anharmonic damped atomic chains

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We investigate the influence of dissipation on envelope solitons on anharmonic chains. We consider both Stokes and hydrodynamical damping and derive the evolution equations for the envelope in both the continuum and the quasi-continuum approximation of the chain. We introduce an appropriate collective variable ansatz for the envelope in order to describe the effect of damping on the soliton shape. We derive ordinary differential equations for the evolution of the three collective variables amplitude, width, and chirp which describe the spatial modulation of the envelope. The analytical results are in good agreement with the simulations of the discrete system for high-energy excitations on the chain. Our results derived from the quasi-continuum approximation show significant improvements compared to the continuum approximation.

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I. INTRODUCTION

Nonlinear one-dimensional lattices bear various interesting phenomena alien to linear physics. Zabusky and Kruskal first recognized in computer experiments that nonlinear coherent excitations propagate in such systems with constant velocity and shape. They coined these solitary waves solitons because they show particle-like behavior, e.g., robustness in scattering among themselves [1]. These pulses are solutions of Boussinesq (Bq) or Korteweg-de Vries (KdV)-type equations (in the long wavelength approximation). The shape of these pulses depends on the interaction potential of the particles whereas realistic interaction potentials always generate a compressive supersonic pulse. Other solutions also exist which possess a rapid internal oscillation; these solutions are called envelope solitons. The nonlinear Schrödinger equation (NLS) governs the evolution of the envelope of the soliton in the continuum description. The excitations with small wave numbers k are called breathers and may be described by a KdV equation [2].

Due to their robust character, the soliton concept is useful in explaining essential features of molecular chains such as the energy transport in polypeptide chains in muscle proteins [3–7] and also the energy transport [8] and the conformational transitions and denaturation [9,10] of the DNA molecule. Especially in the case of biomolecules, damping and thermal fluctuations appear as natural perturbations, but, up to now, the main attention was paid to soliton dynamics in the absence of such perturbations. Recently Arévalo *et al.* investigated the effect of damping and thermal fluctuations on lattice solitons in the quasi-continuum approximation (QCA) where perturbed Bq- or KdV-type equations were used [11,13]. The properties of envelope solitons on a chain connected to a heat bath were discussed in [12]. The envelope solitons were found to possess an anomalous diffusion behavior (superdiffusion) which results from the frailty of the envelope solitons with respect to the damping. Therefore, our aim in the present paper is to focus on the behavior of envelope solitons on damped chains and seek an analytical expression for the time dependence of soliton parameters like amplitude, width, and velocity. We start with the discrete equations for the damped lattice and derive an NLS-type equation with a damping term in the continuum limit when we assume the damping to be small. This type of equation arises in many different fields, e.g., in nonlinear optics, where the NLS describes the behavior of laser beams in optical fibers. The continuum approximation (CA) has fundamental mathematical problems, which were overcome by the quasi-continuum approximation (QCA) of Collins [14] and later by the versions of Rosenau [15] and Hochstrasser *et al.* [3]. With the QCA, one derives well-behaved partial differential equations (PDEs) like the improved Bq (IBq) instead of the Bq equation in the continuum limit of the anharmonic chain. Up to now the QCA according to Hochstrasser *et al.* has been enhanced by Neuper *et al.* [16] for envelope solitons. Our goal is to further expand the QCA to describe a damped chain.

Besides the continuum approximation, a strong tendency to analytically investigate nonlinear discrete systems (see, e.g., [17,18]) arose in recent years. Such systems like nonlinear coupled oscillators can be described by the discrete nonlinear Schrödinger equation (DNLS) which has long been applied in various contexts in physics and biology (e.g., [19] and references therein). Particular attention has been paid to specific solutions of the DNLS, called intrinsic localized modes, or, alternatively, discrete breathers because they are spatially localized and periodic in time.

After introducing the model (Sec. II) and reviewing the calculation of supersonic envelope solitons in the CA and the QCA (Sec. III) of the unperturbed chain, we present in Sec. IV a new evolution equation for an envelope soliton in the QCA of a damped atomic chain. In Sec. V, we describe the influence of the hydrodynamical or Stokes damping on envelope solitons using collective variables, e.g., velocity and

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width, and determine their dynamics both in the CA and the QCA. The comparison of the analytical results with simulations in Sec. VI shows that we are able to describe the shape and behavior of damped envelope solitons for long times and that the results of the QCA are superior in the case of narrow solitons.

We especially emphasize that our theory succeeds in explaining the modulations of the envelope of a damped lattice soliton, a feature which was to our knowledge never observed before for solitons on anharmonic atomic chain models.

II. MODEL

We consider an anharmonic chain of particles with mass M ($M=1$) and an interatomic spacing a ($a=1$). We denote y_n as the longitudinal displacement of the nth particle from its equilibrium position and $\phi_n=y_{n+1}-y_n$ as its relative displacement or strain. The nearest neighbors interact via an interaction potential with a harmonic and a quartic term

$$V(\phi_n)=\frac{\alpha}{2}\phi_n^2+\frac{\gamma}{4}\phi_n^4. \tag{1}$$

For the more general case of cubic and quartic terms, the calculations are similar, yet require a greater technical effort. The stability of the soliton solution in the CA is further reduced by the addition of a cubic term.

We want to allow dissipation in our system and choose Stokes or hydrodynamical damping for every particle n:

$$F_n^{St}=-\nu_{St}\dot{y}_n, \tag{2}$$

$$F_n^{hy}=\nu_{hy}(\dot{y}_{n+1}-2\dot{y}_n+\dot{y}_{n-1}). \tag{3}$$

The Stokes damping corresponds to the situation of a chain in a viscous liquid. In contrast to the Stokes damping, the hydrodynamical damping is an inner mechanism of the system since it depends on the relative motions of the particles. One can easily see that this system obeys the following equations of motion:

$$\ddot{\phi}_n=V'(\phi_{n+1})-2V'(\phi_n)-V'(\phi_{n-1})-\nu_{St}\dot{\phi}_n+\nu_{hy}(\dot{\phi}_{n+1}-2\dot{\phi}_n+\dot{\phi}_{n-1}). \tag{4}$$

We continue with the continuum approximation of this system. Notice that the two damping terms yield a complex dispersion relation [13]. The real part resembles the harmonic dispersion relation of the unperturbed chain. Deviations do occur with both damping mechanisms, although only for small wave numbers k for Stokes and for large wave numbers for hydrodynamical damping. Thus it is problematic to use the Stokes damping for pulse solitons since their spectrum is located at $k=0$, where the Stokes damping causes a dispersion relation with only an imaginary part. This means that the long-wavelength region becomes overdamped with Stokes damping [13]. For envelope solitons we do not expect those problems, since the spectrum is located at the wave number of the carrier wave $k_c>0$.

III. QUASI-CONTINUUM APPROXIMATION

In this section we shortly present the results from the literature and the solutions for envelope solitons in the CA and the QCA which we use as initial conditions of both simulations and theory. The envelope functions of small-amplitude excitations with an internal mode on anharmonic chains are solutions of the NLS [2]. One applies an ansatz representing a narrow-band wave packet on the discrete system with an expansion parameter ϵ and proceeds to the continuum limit only for the envelope functions of the ansatz. This approach is known as the derivative expansion method and was first applied to the anharmonic chain by Tsurui [20]. This procedure uses the multiple scales method where one introduces the new variables $x_i=\epsilon^i x$ and $t_i=\epsilon^i t$. The NLS is the lowest-order equation in ϵ where nonlinear and dispersive terms appear. It is known that the CA exhibits certain mathematical problems. In the case of pulse-shaped excitations the CA leads to a Boussinesq-type equation with an ill-posed initial value problem and the need of additional boundary conditions compared to the discrete problem [15]. The QCA was found to be a more convenient tool to calculate soliton solutions [3,14,15]. Our goal is to show the effect of damping on the envelope soliton. In order to be sure not to miss important effects, we also do not rely on the CA but use the QCA of the chain as a starting point for our calculations. We will occasionally refer to the CA procedure where we especially focus on Ref. [26]. In the case of the QCA, Eq. (4) with $\nu_{St}=\nu_{hy}=0$ is transformed into an operator equation using a full Taylor expansion of the potential terms [$n\to x$, $V'(\phi_{n\pm1})\to e^{\pm\partial_x}V'(\phi(x,t))$]

$$\ddot{\phi}(x,t)=2[\cosh(\partial_x)-1]V'(\phi(x,t)). \tag{5}$$

The QCA for oscillatory excitations was performed by Neuper *et al.* [16] using the procedure of Hochstrasser *et al.* [3] where the QCA is applied to the Fourier transformed equation (5). In [16] an ansatz is given by an expansion into harmonics of $\theta=kn-\omega t$:

$$\phi_n(t)=\sum_{m\in\mathbb{Z}}\chi_m(z)e^{im\theta},\quad \chi_m=\tilde{\chi}_{-m}, \tag{6}$$

where k is the wave number and ω is an amplitude-dependent frequency to be determined later. The envelopes χ_m of the soliton in the QCA move with constant velocity v and therefore depend on the coordinate $z=x-vt$. Inserting the ansatz (6) into (5) and applying the procedure of [3] yields a system of second-order differential equations in z for the envelope functions χ_m (see [16] for details). This system was also used to construct an iterative procedure for the numerical computation of very discrete soliton solutions on chains with arbitrary interaction potentials [16]. For the sake of simplicity, we will restrict ourselves to the case of a quartic anharmonicity because in this case the multiple scale method which was used to approximately solve the equations reduces to only one equation for the first harmonic χ_1. If one uses the normalized soliton velocity $c_o=v/v_h>1$, the solution of $\chi_1=\chi$ determines the bright soliton soliton in the QCA [16]

$$\phi(z,t) = \chi e^{i(kx-c_o\omega_h t)} + \chi e^{-i(kx-c_o\omega_h t)} = 4\frac{\sqrt{c_o^2-1}}{\sqrt{\frac{6\gamma}{\alpha}}}\,\mathrm{sech}\left(2\sqrt{\frac{c_o^2-1}{c_o^2}}z\right)\cdot\cos(kx-c_o\omega_h t+\delta_o), \tag{7}$$

with

$$\omega_h = 2\sqrt{\alpha}\sin\left(\frac{k}{2}\right), \quad v_h = \sqrt{\alpha}\cos\left(\frac{k}{2}\right).$$

Equation (7) has a similar form as the solution of the NLS in the CA [2,12]:

$$\phi(z,t) = \chi e^{i(kx-\omega_h t)} + \tilde{\chi} e^{-i(kx-\omega_h t)} = 4\frac{\sqrt{c_o^2-1}}{\sqrt{\frac{6\gamma}{\alpha}}}\,\mathrm{sech}(2\sqrt{c_o^2-1}z)\cdot\cos(kx-c_o\omega_h t+\delta_o). \tag{8}$$

The widths of the two solutions differ distinctly for large velocities $c_o \gtrsim 1.1$. In this regime the continuum approximation for the envelope begins to fail and the solution (7) achieves better results than (8). An additional cubic term in the potential (1) does not principally change the above procedure but requires a higher technical effort since one has to consider additionally the envelope functions for the harmonics $m=(0,2)$. This extension leads to a solution similar to (7) and (8) with a different amplitude [2,16]. We have not yet considered any damping terms in the QCA. In the case of a damped system, we can no longer assume that the soliton propagates with a permanent profile and a fixed velocity c_o. Therefore, we must consider explicitly time-dependent envelope functions $\chi_m(z(t),t)$ and a time-dependent soliton velocity $v(t)=c_o(t)v_h$ and a dispersion relation $\omega=c_o(t)\omega_h$ (k is still fixed).

IV. QUASI-CONTINUUM APPROXIMATION FOR THE DAMPED SYSTEM

The aim of the present work is to generalize the CA and QCA results to damped systems and so we start with the discrete equations of motion for Stokes ($\nu_{St}>0$, $\nu_{hy}=0$) or hydrodynamical damping ($\nu_{St}=0$, $\nu_{hy}>0$):

$$\ddot{\phi}_n = V'(\phi_{n+1}) - 2V'(\phi_n) + V'(\phi_{n-1}) - \nu_{St}\dot{\phi}_n + \nu_{hy}(\dot{\phi}_{n+1} - 2\dot{\phi}_n + \dot{\phi}_{n-1}). \tag{9}$$

We insert an ansatz such as (6) with explicit time-dependent envelope functions and take into account that the velocity of the soliton could change

$$\phi_n(t) = \sum_{m\in\mathbb{Z}} \chi_m(z(t),t)e^{im\theta}, \quad \chi_{-m} = \tilde{\chi}_m,$$

$$z(t) = n - \int_0^t v(t')dt'. \tag{10}$$

We proceed like in [16], but the coefficients $W_m(z(t),t)$ of the Fourier series for the force $V'(\phi_n)$ become time dependent, since they depend on the envelope functions. Inserting (10) in Eqs. (9) yields the following equations for Stokes damping $[\partial_n \to \partial_z,\ \partial_t \to -v(t)\partial_z + \partial_t]$,

$$[-im\omega(t) - v(t)\partial_z + \partial_t]^2\chi_m(z,t) = 4\sinh\left(\frac{imk+\partial_z}{2}\right)^2 W_m(z,t) + \nu_{St}[v(t)\partial_z + im\omega - \partial_t]\chi_m(z,t), \tag{11}$$

and for hydrodynamical damping

$$[-im\omega(t) - v(t)\partial_z + \partial_t]^2\chi_m(z,t) = 4\sinh\left(\frac{imk+\partial_z}{2}\right)^2 W_m^D(z,t), \tag{12}$$

where

$$\sum_m W_m e^{im\theta} = V'\left(\sum_l \chi_l e^{il\theta}\right),$$

$$W_m^D(z,t) = W_m(z,t) + \nu_{hy}\dot{\chi}_m(z,t) - \nu_{hy} im\omega(t)\chi_m(z,t). \tag{13}$$

The functionals $W_m(z,t)$ depend only on the envelope functions $\chi_l(z,t)$ (13) and collect all terms which belong to the harmonic m. The derivatives $\dot{\omega}$ and $\dot{v}$ are omitted because these terms would drop out when we later calculate the equations in the different orders of ϵ. A rough estimate for the time dependence of c_o gives $\dot{c_o}(t) \sim [c_o(0)-1]\nu \sim \epsilon^4$. As this change of the soliton velocity is so slow, we can treat c_o as a constant parameter in the following steps. The inclusion of the hydrodynamical damping in our scheme is unproblematic, because this damping term has the same symmetry as the potential term. We proceed similarly to the unperturbed case and transform these equations to the Fourier space. For these equations, we must use the space and time Fourier transformations for the envelope functions $\chi_m(z,t)$ and the functionals $W_m(z,t)$

$$f_m(z,t) = \int_\infty^{-\infty}\int_\infty^{-\infty} dq d\Omega \bar{f}_m(q,\Omega)e^{i(qz-\Omega t)}. \tag{14}$$

The variable Ω represents a frequency and appears since our problem became explicitly time dependent. We obtain the following equations for Stokes and hydrodynamical damping in the new coordinates (q,Ω)

$$\bar{W}_m^{St}(q,\Omega) = \underbrace{\frac{\pi_m^2(q,\Omega) + i\nu_{St}\pi_m(q,\Omega)}{4\sinh\left(\frac{mk+q}{2}\right)^2}}_{a_m^{St}(q,\Omega)}\bar{\chi}_m(q,\Omega)$$

$$\bar{W}_m^{hy}(q,\Omega) = \underbrace{\frac{\pi_m^2(q,\Omega)}{4\sinh\left(\frac{mk+q}{2}\right)^2}}_{a_m^{hy}(q,\Omega)}\bar{\chi}_m(q,\Omega)$$

$$\pi_m(q,\Omega) = m\omega + qv + \Omega. \tag{15}$$

As in the CA or QCA, we continue restricting ourselves to small envelope excitations ($\chi_m \sim \epsilon^m$ for $m>0$) and assume the damping to be small ($\nu \sim \epsilon^2$). The spectrum of the soliton should then be located around $(q,\Omega)=(0,0)$. Therefore, we may proceed with a Taylor expansion of the functions $a_m^{St/hy}(q,\Omega)$:

$$a_m(q,\Omega) = a_{(0,0),m} + a_{(1,0),m}q + a_{(0,1),m}\Omega + a_{(2,0),m}q^2 + a_{(0,2),m}\Omega^2 + a_{(1,1),m}q\Omega + \cdots. \tag{16}$$

After this approximation, we transform the equations (15) back to the position space. As mentioned before for the unperturbed system, only the envelope functions $\chi_{\pm 1}$ are nonzero in case of an interaction potential with only a quartic anharmonicity ($m=\pm 1$). Because of the stipulation $\chi_1 \sim \epsilon$, it was pointed out in [16] that it is reasonable to assume that the derivative ∂_z enters the equations in $\mathcal{O}(\epsilon)$. Since the damping constant ν was specified to be in order $\mathcal{O}(\epsilon^2)$, we assume that the time derivative of the envelope appears in the same order. If we apply these assumptions to our previous results, we can neglect the terms for $a_{(1,1),\pm 1}$ and $a_{(0,2),\pm 1}$ which appear in a higher order than $\mathcal{O}(\epsilon^3)$. Taking into account the concrete form of $a_{\pm 1}^{St/hy}(q,\Omega)$, we can now calculate the explicit expressions for the remaining Taylor coefficients and the dispersion relations for the two different damping mechanisms ($m=\pm 1$):

$$a_{(0,0)}^{St/hy} = \frac{\alpha v^2}{v_h^2} + \mathcal{O}(\nu_{St}^2) = \alpha c_o(t)^2 + \mathcal{O}(\nu_{St}^2), \tag{17}$$

$$a_{(0,1)}^{St/hy} = \frac{2c_o(t)\alpha}{\omega_h}, \tag{18}$$

$$a_{(2,0)}^{St/hy} = \frac{\alpha c_o(t)^2}{4} + \mathcal{O}(\nu_{St}^2), \tag{19}$$

$$\omega^{St} = c_o(t)\omega_h(k) - mi\frac{\nu_{St}}{2} + \mathcal{O}(\nu_{St}^2), \tag{20}$$

$$\omega^{hy} = c_o(t)\omega_h(k). \tag{21}$$

The dispersion relations are calculated by assuming $a_{(1,0),1}=0$ as done in [3,16] for the undamped chain. Inserting (17)–(21) in (15) and transforming back to the (z,t) space results in the following modified NLS (mNLS) equation for the envelope $\chi(z,t)=\chi_1(z,t)$:

$$i\partial_\tau\chi + i\Gamma_{St/hy}\chi + c_o(\tau)\partial_z^2\chi + \frac{\kappa}{c_o(\tau)}|\chi|^2\chi - 4\frac{c_o(\tau)^2-1}{c_o(\tau)}\chi = 0, \tag{22}$$

where

$$\tau = -\frac{\omega_h}{8}t, \quad \kappa = \frac{12\gamma}{\alpha},$$

$$\Gamma_{hy} = -\frac{4\nu_{hy}\omega_h}{\alpha}, \quad \Gamma_{hy} = -\frac{4\nu_{St}}{\omega_h}. \tag{23}$$

The envelope function $\chi_{-1}=\tilde{\chi}$ obeys the c.c. mNLS (22). This equation looks similar to a damped NLS. If the additional parameter $c_o(t)$, the normalized velocity of the envelope soliton, is close to 1, the equation (22) then corresponds to the damped NLS we would obtain in the CA.

In the next section, our goal is to investigate the properties of the damped envelope soliton. We perform a collective variable approach for the equation (22) in terms of a chirped trial function, which was found to be a good ansatz to analyze NLS-type equations [22]:

V. COLLECTIVE VARIABLE APPROACH

In the case of a damped NLS [(22) with $c_o \to 1$] and the mNLS [(22) with $c_o > 1$], it is convenient to use a variational analysis since it is easy to find the Lagrange densities $\mathcal{L}$ for these equations. One only must insert a trial function with several collective variables (CVs) in the Lagrange density and calculate the Lagrangian L by a spatial integration. One can then minimize the action according to the Hamiltonian principle with respect to the time-dependent CV $x_i(t)$ of the trial function,

$$\frac{d}{d\tau}\frac{\partial L}{\partial x_{i\tau}} - \frac{\partial L}{\partial x_i} = 0, \tag{24}$$

in order to obtain a set of ordinary differential equations (ODEs) for the CV. One could also apply other methods like the projection method [23,24] or a perturbation scheme based on the inverse scattering theory for the NLS [25]. But in this context we are sure that the shape of the CV ansatz and the number of CVs are the items which decide on the results rather than the perturbation procedure itself. A similar procedure was used in nonlinear optics for the NLS [22,26] but to our knowledge never in the context of lattice solitons within the framework of the QCA. For the mNLS (22) we can find a Lagrange density for either Stokes $\Gamma=\Gamma_{St}$ or hydrodynamical damping $\Gamma=\Gamma_{hy}$

$$\mathcal{L} = \exp(2\Gamma\tau)\left[\Im(\tilde{\chi}\chi_\tau) + c_o(\tau)|\chi_z|^2 - \frac{\kappa}{2c_o(\tau)}|\chi|^4 - \frac{4(c_o(\tau)^2-1)}{c_o(\tau)}|\chi|^2\right]. \tag{25}$$

The crucial point in the variational analysis of the mNLS

(22) is the role of the parameter c_o, which is the normalized velocity of the envelope soliton which we do not have in the corresponding NLS equation (limit $c_o \to 1$). We present a CV ansatz which slightly differs from the ansatz in [22,26]:

$$\chi = A(\tau)\mathrm{sech}\left(\frac{z - Z(\tau)}{B(\tau)}\right) \cdot \exp\left(\pm i\alpha(\tau)z^2 \pm iQ(\tau)[z - Z(\tau)]\right). \tag{26}$$

For the damped NLS in the CA one would have to use an additional phase which takes a similar role as c_o does here in the QCA. The amplitude A, width B, and chirp factor α are used as collective variables. The CV α enables a z-dependent spatial modulation of the envelope function $\chi(z,t)$ (chirp). The two CVs Q and Z were added to enable a center of mass motion for the envelope soliton relative to the coordinate $z(t)$ (10), but they do not evolve in time when initialized with zero $[Q=Q(0)=Z=Z(0)=0]$.

If we insert this ansatz in the Lagrange density, calculate the Lagrangian, and minimize with respect to the CV in the ansatz, we obtain the following system:

$$N(t) = N_o \exp\left(2\Gamma \frac{w_h}{8} t\right), \tag{27}$$

$$\frac{dB}{dt} = -\frac{\omega_h}{2} c_o(t)\alpha(t)B(t), \tag{28}$$

$$\frac{d\alpha}{dt} = -\frac{\omega_h}{2} c_o(t)\left(\frac{1}{4B^4}\frac{4}{\pi^2} - \alpha^2\right) + \frac{2\kappa}{\pi^2 c_o(t)}\frac{A^2}{B^2}, \tag{29}$$

$$c_o(t)^2 = \frac{1}{1 + 6B(t)^2}\left(\frac{10\kappa A(t)^2 B(t)^2}{8} + 6B(t)^2\right), \tag{30}$$

$$N_o = 2B_o A_o^2 = \frac{2c_o(0)\sqrt{c_o(0)^2 - 1}}{3},$$

$$B_o = \frac{2\sqrt{c_o(0)^2 - 1}}{c_o(0)}, \quad \alpha(0) = 0.$$

For $c_o(0) \to 1$, the equations (28) and (29) correspond to the equations in the CA calculated by Rasmussen *et al.* [26] in the context of the critical collapse in the NLS with arbitrary degree of nonlinearity σ. The derived equations for the CVs in the QCA (and the CA) can be solved numerically [27] and compared with the simulations of the discrete system.

VI. SIMULATIONS

It is now time to compare the results of the CV analysis with the simulations of the original, discrete system. First we discuss the algorithm of the time integration and the numerical routines to find the position, norm, and amplitude. Then we compare the simulation results with the solution of the ODEs for the CVs in the last section.

A. Algorithm

The discrete equations of motion for the anharmonic chain with N particles in relative coordinates read

$$\ddot{\phi}_n = \alpha[\phi_{n+1} - 2\phi_n + \phi_{n-1}] + \gamma[\phi_{n+1}^3 - 2\phi_n^3 + \phi_{n-1}^3] - \nu_{St}\dot{\phi}_n + \nu_{hy}(\dot{\phi}_{n+1} - 2\dot{\phi}_n + \dot{\phi}_{n-1}), \tag{31}$$

where we always choose $\alpha=\gamma=1$ in the simulations. At $t=0$, the chain is initialized by a discrete version of the envelope soliton (8) and (7). We choose periodic boundary conditions in order to be able to run long simulations,

$$\frac{d^l\phi_0}{dt^l} = \frac{d^l\phi_{N-1}}{dt^l}, \quad \frac{d^l\phi_N}{dt^l} = \frac{d^l\phi_1}{dt^l}, \quad l = 0,1. \tag{32}$$

We use relative coordinates because in this representation the amplitude of the envelope soliton vanishes at infinity. The simulations are performed for a chain with at least 1000 lattice points. The time integration is carried out by using the Heun method [28] which was successfully used for the numerical solution of partial differential equations and difference-differential equations, coupled to either an additive or a multiplicative noise term [29–32]. The initial condition for the chain at $t=0$ is presented in Fig. 1(a) together with a snapshot of the chain at a later time t [Fig. 1(b)] which is comparable to $\bar{t} = \nu_{St}^{-1} t = 1$. One can see that the damping has a large effect on the shape of the soliton. The amplitude of the soliton decreases while the width shows a clear increase for these times. In order to detect the position of the soliton we search for the center of the norm M of the envelope soliton. In the continuum description the norm M is a conserved quantity for the unperturbed soliton as it results to be twice the norm N of the envelope:

$$M = \int_{-\infty}^{\infty} \phi(x,t)^2 dx \overset{(8)}{\approx} 2\int_{-\infty}^{\infty} |\chi(x,t)|^2 dx = 2N_o. \tag{33}$$

In the simulations we identify M with a discrete sum over the core of the envelope, although the discreteness effects are negligible for low-energy solitons ($c_o - 1$ small). We define the soliton position $x_s(t)$ as the center of the norm or mass M of the envelope soliton

$$x_s(t) = \frac{\sum_{i=n_1}^{n_2} i\phi_i^2}{\sum_{i=n_1}^{n_2} \phi_i^2}, \tag{34}$$

where the integers n_1 and n_2 mark the core of the envelope and depend on the position of the soliton and its width at the last time step.

We use the quantity $\phi(x_s(t))$, the relative displacement of the soliton position, to estimate the amplitude $\mathcal{A}$ of the damped soliton, since $\phi(x_s(t))$ takes values in the range $[+\mathcal{A}, -\mathcal{A}]$. After typical times of a few $\bar{t}$, the amplitude of the envelope soliton (in relative coordinates) becomes very small compared with that of the start soliton. For pulse solitons, it takes much longer times $\bar{t}$ until the soliton disappears. The physical picture which explains the strong influence of the damping on the envelope soliton is the rapid motion of the particles in the profile of the envelope due to the internal mode. The particles in the profile of a pulse soliton move much slower and therefore dissipate less energy.

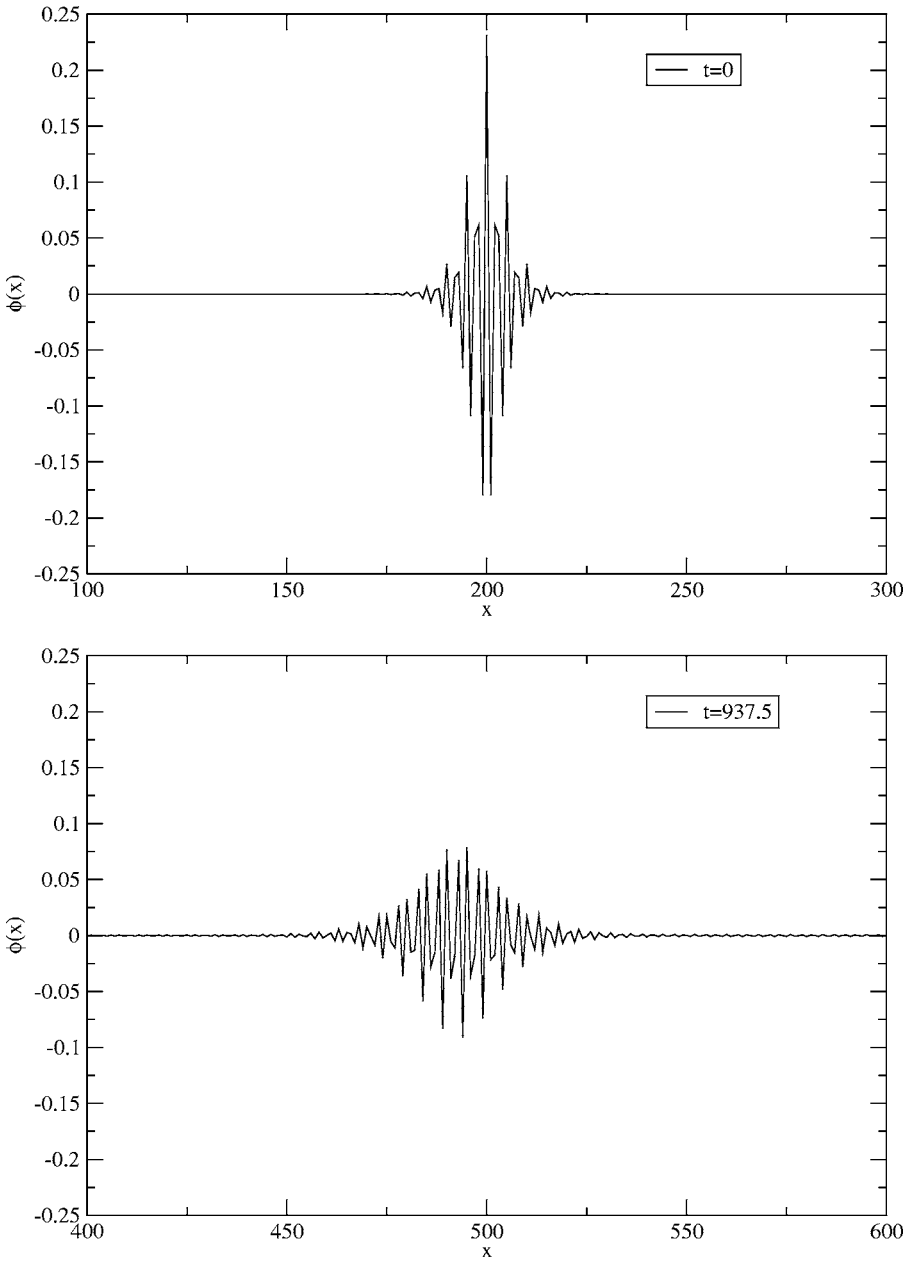

FIG. 1. Envelope soliton ($k=4\pi/5$, $c_o=1.01$) on a damped chain ($\nu_{St}=0.001$).

B. RESULTS

We will test the quality of our theory by the results of the simulations of the discrete system. First of all we can check the predicted behavior for the norm of the soliton $M(t)$. It has been known for a long time that the norm M of the damped envelope soliton decreases exponentially ($\sim e^{-2\Gamma\tau}$) [25]. This decrease means that the norm of the soliton decays like $M \sim e^{-\nu_{St}t}$ for the Stokes damping and like $M \sim e^{-2\nu_{hy}[1-\cos(k)]}$ for the hydrodynamical damping. If the discreteness effects are negligible (c_o-1 small), the norm of the soliton, measured in the simulations, should show an exponential decrease.

As one can see in Fig. 2(a), this property is fulfilled for both the Stokes and the hydrodynamical damping. The damping rate of the norm in the case of hydrodynamical damping is k dependent and is plotted in Fig. 2(b) for three different wave numbers $k=\{0.4\pi,0.6\pi,0.8\pi\}$. The agreement with the theoretical prediction is very good, except for the smallest value of the wave number ($k=0.4\pi$), where the theoretical curve begins to differ from the simulation results. This deviation occurs for small wave numbers since the carrier wavelength λ_c is no longer distinctly smaller than the envelope width λ_e, a condition which was used in the multiple scale method to derive the NLS-type equations. The quantity $M(t)$ may be used to estimate whether the continuum approximation is appropriate. For the parameter range ($c_o>1.1, k\to 0$) the theory is unable to produce good agreement with the simulations since the underlying multiple scale scheme fails.

We focus on the differences between the predictions for the CV in the continuum and the quasi-continuum approximation of the damped chain. Therefore, we will compare the results $\phi(x_s)$ from the simulations with the behavior for the

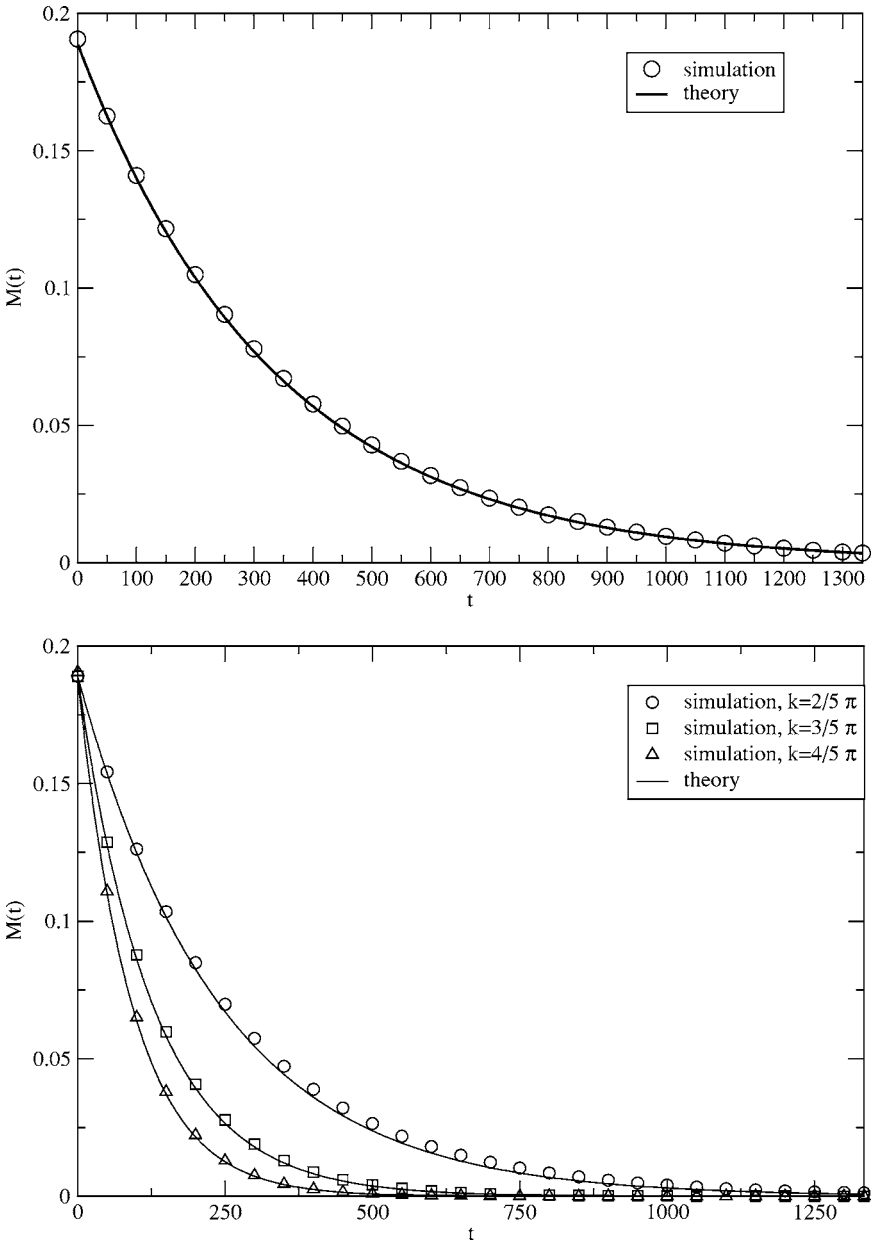

FIG. 2. Norm of an envelope soliton ($k=4\pi/5$, $c_o=1.01$) on a damped chain for either Stokes or hydrodynamical damping [(a) $\nu_{St}=0.003$, $\nu_{hy}=0$, (b) $\nu_{St}=0$, $\nu_{hy}=0.003$].

soliton amplitude $\mathcal{A}=2A$ of the CV theory. For low-energy excitations ($c_o\rightarrow 1$) the QCA should produce the same results as the CA since the mNLS (22) passes into the NLS, but we expect differences for high-energy excitations, where the continuum approximations begin to fail, because the envelope becomes very narrow. One should keep in mind that a normalized velocity such as $c_o=1.1$ corresponds to a very narrow envelope (width $B\approx 1$) in relative coordinates. In Fig. 3 we plot only the positive values of $\phi(x_s)$ which is the relative displacement at the soliton center. It is obvious that the maxima of $\phi(x_s)$, which indicate the amplitude of the lattice soliton in the simulations, show good agreement with the QCA results. We use a chain with Stokes damping in Fig. 3, since narrow envelope solitons show certain instabilities in the presence of hydrodynamical damping. These instabilities occur since the hydrodynamical damping term is mathematically more complex and yields a larger number of higher-order terms in ϵ, which are not considered by our theory.

We return to smaller and broader envelope solitons, where the continuum and the quasi-continuum approximation are appropriate. We want to demonstrate the agreement between our theory and the simulations for one more example. We consider an envelope soliton with $k=\pi$ on a damped chain ($\nu_{St}=0.003$) of atoms. This soliton is immobile since $v_h(\pi)=0$ and can be compared with results in Ref. [16] for an undamped chain. After typical times of a few $\bar{t}$ the envelope of the soliton begins to develop spatial modulations which are symmetric with respect to the soliton position $x_s(t)=x_s(0)$. In Fig. 4, we take a snapshot of the chain at time $t=1400>4/\nu_{St}$. Additionally, we plot the theoretical prediction of the soliton shape, where we use the results of the numerical solution of the equations (27)–(30) for the CVs α, A, and B at time $t=1400$. Every particle is situated on the envelope of the soliton since the factor $\cos(\pi n)$ only yields multiplicative constants $(-1)^n$ for the discrete variable n.

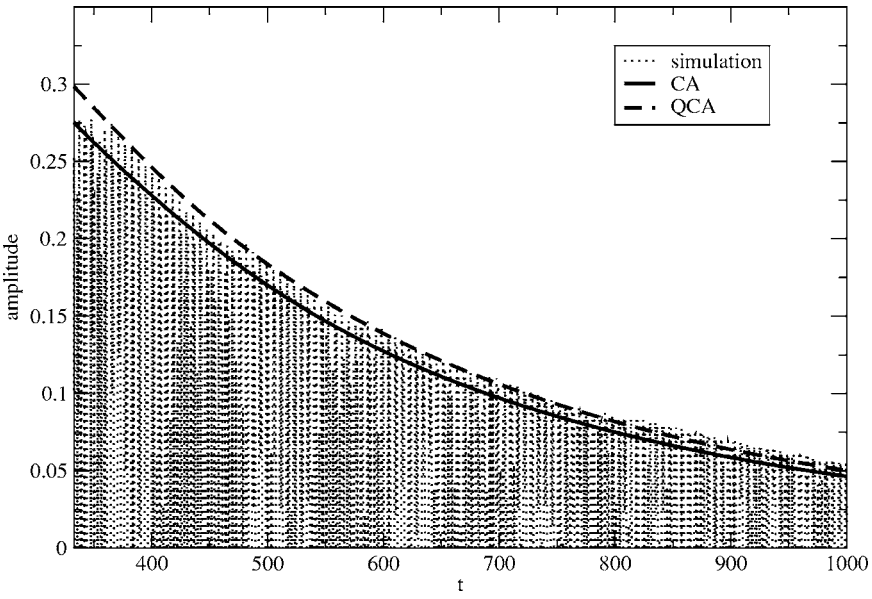

FIG. 3. Amplitude comparison of an envelope soliton ($k=4\pi/5$, $c_o=1.1$) on a damped chain ($\nu_{St}=0.003$). The results for the collective variable $\mathcal{A}=2A$ in the CA and the QCA as well as the quantity $\phi(x_s)$ from the simulations are displayed. In order to show the slight differences we only present the positive values of $\phi(x_s)$ in a time interval $1/2\nu_{St}<t<3/\nu_{St}$.

The agreement with the theory is very convincing, considering the fact that the snapshot in Fig. 4 is taken at a time when the soliton has almost disappeared. There are only minor deviations for large times in the tails of the envelope, which could imply that the hyperbolic secans which results from the unperturbed problem is not the perfect choice as a trial function. The results for other wave numbers tend to be less precise than they are in Fig. 4, nevertheless they are still in good agreement with the simulations.

VII. CONCLUSIONS

In the present work we have generalized the QCA for envelope solitons on anharmonic lattices for the cases of Stokes and hydrodynamical damping. We have extended the QCA for envelope solitons [16] to the damped chain and derived a modified damped NLS-type equation (mNLS) to be the evolution equation of the envelope. We applied a similar analysis as for the damped NLS [22,26] and found that the mNLS is superior in the case of high-energy excitations when the envelope becomes very narrow. The crucial point of the applied method is the application of a chirped trial function (26) for the damped envelope soliton. If one would use the bright soliton solution as an ansatz (like in [12]), one would omit the effects of the spatial envelope modulations (Fig. 4). Moreover, the adiabatic ansatz would describe the dynamics of the amplitude and the width using only one CV $\eta(t)$. The adiabatic ansatz forces an exponentially decreasing amplitude and an exponentially increasing width, which has long been known to be correct only for small times compared with the inverse damping constant ($t \ll \nu^{-1}$).

In conclusion, we can recapitulate that the combination of an adequate CV ansatz, which in the case of a damped envelope soliton means the inclusion of a chirped trial function, with the QCA of the discrete system leads to a very good

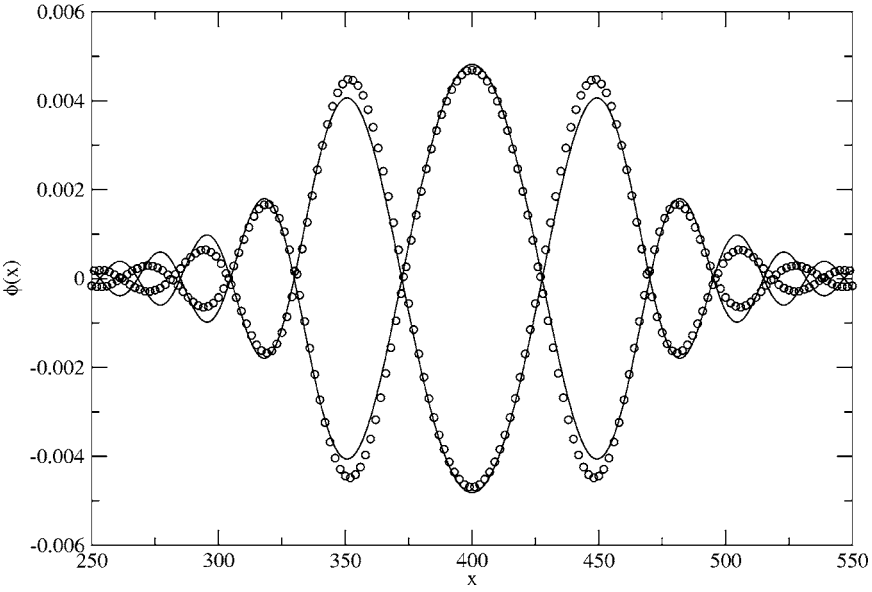

FIG. 4. Snapshot of an envelope soliton ($k=\pi$, $c_o=1.01$) on a damped chain ($\nu_{St}=0.003$) compared to the theoretical prediction (solid line) at time $t=1400$. Here the results of the numerical solution of Eqs. (27)–(30) were used.

agreement between simulations and analytical predictions. The QCA approximation is essential in the case of very narrow solitons and in our opinion results to be more elegant than, e.g., a continuum approximation with the inclusion of higher-order terms for the same purpose. The chirping of approximate NLS solutions was a well-known fact in the literature and we reported it in relation to solitons on damped FPU chains.

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