Eur. Phys. J. B **42**, 103–112 (2004)
DOI: 10.1140/epjb/e2004-00361-0

**THE EUROPEAN PHYSICAL JOURNAL B**

# Thermal diffusion of envelope solitons on anharmonic atomic chains

C. Brunhuber[1,a], F.G. Mertens[1], and Y. Gaididei[2]

[1] Physikalisches Institut, TP 1, Universität Bayreuth, 95440 Bayreuth, Germany
[2] Bogolyubov Institute for Theoretical Physics, 03143 Kiev, Ukraine

Received 28 June 2004
Published online 26 November 2004 – 

**Abstract.** We study the motion of envelope solitons on anharmonic atomic chains in the presence of dissipation and thermal fluctuations. We consider the continuum limit of the discrete system and apply an adiabatic perturbation theory which yields a system of stochastic integro-differential equations for the collective variables of the ansatz for the perturbed envelope soliton. We derive the Fokker-Planck equation of this system and search for a statistically equivalent system of Langevin equations, which shares the same Fokker-Planck equation. We undertake an analytical analysis of the Langevin system and derive an expression for the variance of the soliton position $Var[x_s]$ which predicts a stronger than linear time dependence of $Var[x_s]$ (superdiffusion). We compare these results with simulations for the discrete system and find they agree well. We refer to recent studies where the diffusion of pulse solitons were found to exhibit a superdiffusive behaviour on longer time scales.

**PACS.** 05.10.Gg Stochastic analysis methods – 05.45.Yv Solitons – 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 05.50.+q Lattice theory and statistics

## 1 Introduction

Anharmonic one-dimensional lattices play an important role in physics. Since the first computer based numerical investigations physicists have known that coherent excitations propagate in such systems with constant velocity and shape. Zabusky and Kruskal showed in computer experiments that these excitations were robust in scattering among themselves, thus they coined them "solitons" [1]. Numerical simulations of chains at finite temperature with realistic interaction models such as the Lennard-Jones potential showed that these compressive and supersonic pulses propagate over long distances [2]. The soliton concept is thus useful in explaining essential features of molecular chains, such as the energy transport in $\alpha$-helical proteins [2–5]. Nonlinear lattice dynamics may be applied to model the energy transport in DNA molecules [6] as well as the denaturation and conformational transitions in the DNA [7,8]. Unfortunately no exact soliton solutions exist for the continuum approximation (CA) of atomic chains with realistic interaction potentials like the Lennard-Jones or Morse potential. Therefore, analytical studies of nonlinear lattice dynamics are primarily based on chains possessing cubic and/or quartic anharmonicity. In this case the CA yields Boussinesq (Bq) or Korteweg-de Vries (KdV) type equations. If one assumes soliton solutions with an internal oscillation, the CA yields a Nonlinear Schrödinger equation (NLS) for the envelope of the soliton [9].

Though these facts have been known for quite some time there exist few publications on soliton dynamics in *perturbed* lattice models. In the case of biomolecules, especially damping and thermal fluctuations appear as natural perturbations. Recently Arévalo et al. investigated the dynamics of pulse solitons on an atomic chain with cubic anharmonicity in the presence of damping and noise [10]. The damping and noise terms satisfy the fluctuation-dissipation theorem where the noise is assumed to be Gaussian white noise. The analytical results are compared with the results of Langevin dynamics simulations of the chain. The position and the inverse width of the soliton solution were found to be good collective variables (CV) for the perturbed soliton. The correlation between the shape and the velocity of the pulse solitons leads to an anomalous variance of the soliton position $Var[x_s]$. For longer time intervals, $Var[x_s]$ of the pulse solitons grows stronger than linearly in time (superdiffusion). This effect was also observed in the case of pulse solitons in classical Heisenberg chains [11].

Here, we investigate the diffusion of envelope solitons, the second class of non-topological solitons, in order to determine whether superdiffusion is a generic behaviour for these excitations.

In this article, we present the effects of damping and thermal fluctuations on the propagation of the envelope

[a] e-mail: Christian.Brunhuber@uni-bayreuth.de

solitons. We proceed similarly as above and describe the perturbed envelope of the soliton by the bright soliton solution and derive Langevin equations for the 2 CV.

## 2 Model

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

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

For the more general case of cubic and quartic terms, the calculations are similar yet require a greater technical effort. In this case the range of validity for the theory would also be smaller since one must then consider higher harmonic terms in (8).

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

$$F_n^{St} = -\nu_{St}\dot{y}_n. \quad (2)$$

The Stokes damping corresponds to the situation of a chain in a viscous liquid. In contrast to the hydrodynamical damping, which is an inner mechanism of the system, the Stokes damping does not change the dispersion relation of plane waves $\omega_h(k)$ with sufficiently large wave numbers k. This fact is important for the derivation of the NLS in the next section. The noise term, for this damping, which fulfils the fluctuation-dissipation theorem takes the simple form

$$F_n^N(t) = \sqrt{D}\xi_n(t), \quad (3)$$

where

$$D = 2\nu_{St}k_BT \quad (4)$$

is the diffusion constant, $k_B$ is the Boltzmann constant and $T$ is the temperature of the thermal bath. We assume $\xi_n(t)$ to be delta-correlated white noise

$$\langle \xi_n(t)\xi_m(s)\rangle = \delta_{nm}\delta(t-s) \quad (5)$$

$$\langle \xi_n(t)\rangle = 0. \quad (6)$$

It is easy to show that this system obeys the following equations of motion

$$\ddot{y}_n = V_n' - V_{n-1}' - \nu_{St}\dot{y}_n + \sqrt{D}\xi_n(t). \quad (7)$$

## 3 Continuum approximation

Since the discrete equations of motion can not be solved analytically, we go on with a continuum approximation where we assume that the envelope width is much larger than the lattice constant. It has long since been documented that the envelope of small-amplitude excitations with an internal mode on anharmonic chains are NLS solutions [9]. It is suggesting to study the dynamics of the perturbed soliton by a collective coordinate approach for the envelope similar to the bright soliton solution of the NLS. One derives the NLS equation in absolute displacement coordinates if one looks for solutions

$$y_n = \sum_l \epsilon^l \sum_m F_{l,m}e^{im\theta} + \text{c.c.} \quad (8)$$

with the phase $\theta = kn - \omega t$ and only assuming the continuum limit for the envelope functions $F_{l,m}$. This approach is known as the reductive perturbation method and was first applied to the anharmonic chain by Tsurui [12]. For the quartic potential, only the terms for $l = 1$ and $m = 1$ contribute. Thus, the following ansatz suffices

$$y_n(t) = F_n(t)e^{i\theta} + \tilde{F}_n(t)e^{-i\theta}\ ,\ F_n \sim \epsilon. \quad (9)$$

The reductive perturbation technique is accompanied by the multiple scale method. After substituting (9) in the equation of motion and assuming the continuum limit for the envelope function ($F_n(t) \to F(x,t)$)

$$F_{n\pm1} = F \pm \partial_x F + \partial_x^2 F + ..., \quad (10)$$

one introduces the new variables $x_i = \epsilon^i x$, $t_i = \epsilon^i t$ and analyses the equations in the different orders of $\epsilon$. In the first order $\mathcal{O}(\epsilon^3)$, where nonlinear terms and the damping ($\nu_{St} \sim \epsilon^2$) begin to contribute, one obtains an NLS in the new coordinates $\tau = -\frac{\omega_h}{4}t$ and $z = (x - x_o) - vt$ with a damping term $i\Gamma F$

$$i\partial_\tau F + \frac{1}{2}\partial_z^2 F + \kappa \mid F \mid^2 F + i\Gamma F = 0, \quad (11)$$

where $\omega = \omega_h = 2\sqrt{\alpha} \mid \sin(\frac{k}{2}) \mid$, $\kappa = 6\frac{\gamma\omega_h^2}{\alpha^2}$ and $\Gamma = -\frac{2\nu_{St}}{\omega_h}$. The evolution equation of the conjugated complex (c.c.) envelope $\tilde{F}$ is the c.c. of the NLS (11). In order to include the noise term in this scheme, it is useful to use a similar ansatz for the noise

$$\xi_n(t) = \frac{1}{2}\Big[\Xi_n(t)e^{i\theta} + \tilde{\Xi}_n(t)e^{-i\theta}\Big], \quad (12)$$

where $\Xi_n(t) = \xi_n^a(t) + i\xi_n^b(t)$. If $\xi_n^a(t)$ and $\xi_n^b(t)$ are white noises, delta-correlated in space and time, the conditions (5) and (6) for $\xi_n(t)$ are still valid. The new noise term $\Xi(x,t)$ will appear in the NLS if we assume the temperature to be in the order $k_BT \sim \epsilon^4$ ($\sqrt{D} \sim \epsilon^3$)

$$i\partial_\tau F + \frac{1}{2}\partial_z^2 F + \kappa \mid F \mid^2 F = iR\ , \quad (13)$$

with $R = -\Gamma F - i\frac{\sqrt{D}}{\omega_h^2}[\xi^a(x,t) + i\xi^b(x,t)]$. The bright soliton solution of the NLS ($R = 0$) is

$$F(\tau,z) = \frac{\eta_o}{\sqrt{\kappa}}\text{sech}[\eta_o(z+\zeta_o\tau)]e^{-i\zeta_o z + i(\frac{\eta_o^2}{2} - \frac{\zeta_o^2}{2})\tau}, \quad (14)$$

which corresponds to the envelope soliton (9)

$$y(z,t) = \frac{4\sqrt{c_o^2-1}}{\sqrt{\kappa}}\mathrm{sech}\left[2\sqrt{c_o^2-1}z\right] \times \cos(kx - c_o\omega_h t), \quad (15)$$

where we substituted the parameter $\eta_o$ with the normalized velocity $c_o = \sqrt{\frac{\eta_o^2}{4}+1}$. $\zeta_o$ is initially chosen as zero because it only takes the role of an additional velocity relative to the $z$-coordinate. The normalized velocity $c_o$ is restricted to values nearly equal to one since we assumed $\eta_o$ to be in $\mathcal{O}(\epsilon)$. The second free parameter of the envelope soliton is the wavenumber $k$ of the internal mode. It should not be too small because the multiple scale scheme is only a good approximation if the envelope functions vary distinctly slower on the chain than the internal oscillation. In relative coordinates the envelope soliton solution $\phi(x,t) = Ge^{i\theta} + \tilde{G}e^{-i\theta}$ differs from the solution (15) in absolute coordinates due to a different nonlinearity $\kappa = \kappa_r = \frac{6\gamma}{\alpha}$. That is why the equivalent procedure in relative coordinates also yields a NLS similar to (13) for the envelope function $G(x,t)$. In the following section we will discuss the perturbative effects on the soliton which are caused by both the damping and the noise term. For envelope solitons it is convenient to choose Stokes damping which is not possible in the case of pulse solitons since the long-wavelength region ($k \sim 0$) becomes overdamped [13]. Aside from the fact that the Stokes damping yields a very simple noise term, there are two even more important reasons to prefer Stokes damping. The first reason is because the hydrodynamical damping depends on the relative motions of the particles

$$F_n^{hy} = \nu_{hy}(\dot{y}_{n+1} - 2\dot{y}_n + \dot{y}_{n-1}), \quad (16)$$

which yields a $k$-dependent damping term in the NLS (11) ($\nu_{St} \to 2\nu_{hy}[1-\cos(k)]$). As a consequence of the CA, we are restricted to larger values of $k$ which cause larger effective damping rates. This effect is obstructive since our goal is to investigate the soliton diffusion. The second reason why Stokes damping is preferred is because the hydrodynamical damping term is mathematically more complex yielding higher order terms $\mathcal{O}(\epsilon^j)$ with $j > 3$ in the CA which limits the validity range of the theory.

## 4 Adiabatic perturbation theory

Now we investigate the effect of damping and noise in the perturbed NLS (13) with an adiabatic perturbation theory. Similar problems appear e.g. in the field of nonlinear optics where the NLS describes the propagation of a laser beam in an optical fiber. Phenomena such as a fluctuating nonlinear dielectric permittivity, a deviating fiber radius, stationary inhomogeneous media or a random initial shape of the pulse may also be described by different stochastic terms in the perturbation term $R$. In contrast to (13), the random perturbations in nonlinear optics appear most often as multiplicative noise terms [14,15]. The adiabatic perturbation theory presumes that the perturbation term $R$ in (13) is sufficiently small and the envelope of the soliton can be approximated by the bright soliton solution of the NLS. This approach is not the optimal choice if one is interested in the noise-induced effects on the amplitude or the width of the soliton. In the case of a damped soliton the dynamics of the amplitude and the inverse width are decoupled and can no longer be modeled by a single collective coordinate like in (15). The adiabatic approach only yields good results for small time frames which was proven by numerical solutions and analytical investigations of the damped NLS (11). In this case we are mainly interested in the diffusive behaviour of the soliton and we attempt to investigate this fastidious problem with an simple approach. The parameters of the soliton in the adiabatic perturbation scheme, namely amplitude and velocity, are no longer constants. They are assumed to be time-dependent due the perturbation terms in (13)

$$F(\tau,z) = \frac{\eta(\tau)}{\sqrt{\kappa}}\mathrm{sech}[\eta(\tau)(z - z_o(\tau))]e^{-i\zeta(\tau)z + i\sigma(\tau)}, \quad (17)$$

where $z_o(t)$ and $\sigma(t)$ are expressions which depend on $\eta(t)$ and $\zeta(t)$

$$\frac{dz_o}{d\tau} = -\zeta(\tau) \quad (18)$$

$$\frac{d\sigma}{d\tau} = \frac{1}{2}\left(\eta(\tau)^2 - \zeta(\tau)^2\right). \quad (19)$$

In order to determine the time dependence of the collective variables $\eta(t)$ and $\zeta(t)$ one can use the conserved quantities of the NLS. For $R = 0$ the norm $\mathcal{M}$ and the momentum $\mathcal{P}$ are conserved for the NLS field F

$$\mathcal{M} = \int_{-\infty}^{\infty} |\, F \,|^2 \, dz = \frac{2\eta_o}{\kappa} \quad (20)$$

and

$$\mathcal{P} = \int_{-\infty}^{\infty}\left[\tilde{F}_z F - \tilde{F}F_z\right]dz = -\frac{2\eta_o\zeta_o}{\kappa}. \quad (21)$$

For $R \neq 0$ the norm and momentum of the envelope depend on time

$$\frac{\partial\mathcal{M}}{\partial\tau} = \int_{-\infty}^{\infty}\left[F\tilde{R} + \tilde{F}R\right]dz \quad (22)$$

$$\frac{\partial\mathcal{P}}{\partial\tau} = \int_{-\infty}^{\infty}\left[\tilde{F}_z R - F_z\tilde{R}\right]dz. \quad (23)$$

Comparing (20) with (22) and (21) with (23) one can immediately specify the equations for the time dependence for the collective variables $\eta(t)$ and $\zeta(t)$

$$\frac{d\eta}{d\tau} = \frac{\kappa}{2}\int_{-\infty}^{\infty}[F\tilde{R} + R\tilde{F}]dz \quad (24)$$

$$\frac{d\zeta}{d\tau} = -\frac{i\kappa}{2\eta}\int_{\infty}^{\infty}[\tilde{F}_z R - F_z\tilde{R}]dz - \frac{\zeta}{\eta}\frac{d\eta}{d\tau}. \quad (25)$$

Inserting (13) and (17) in (24) and (25), one shows that the CV fulfil the following system of stochastic integro-differential equations:

$$\begin{pmatrix} \dot{\eta} \\ \dot{\zeta} \\ \dot{\sigma} \\ \dot{z_o} \end{pmatrix} = \begin{pmatrix} -2\Gamma\eta \\ 0 \\ \frac{1}{2}(\eta^2 - \zeta^2) \\ -\zeta \end{pmatrix} + \int_{-\infty}^{\infty} dz \begin{pmatrix} B_{11} & B_{12} & 0 & 0 \\ B_{21} & B_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \xi^1 \\ \xi^2 \\ \xi^3 \\ \xi^4 \end{pmatrix} \tag{26}$$

where a dot denotes the derivative with respect to $\tau$. The noise vector $\boldsymbol{\xi}$ consists of white noise components

$$\left\langle \xi^i(t)\xi^j(s) \right\rangle = \delta_{ij}\delta(t-s), \tag{27}$$

where $\xi^1$ and $\xi^2$ adopt the role of $\xi^a$ and $\xi^b$ in (13). The diffusion terms read

$$B_{11} = -\Delta\eta\sqrt{\kappa}\text{sech}[\psi]\sin(\Psi) \tag{28}$$

$$B_{12} = -\Delta\eta\sqrt{\kappa}\text{sech}[\psi]\cos(\Psi) \tag{29}$$

$$B_{21} = \Delta\eta\sqrt{\kappa}\text{sech}[\psi]\tanh[\psi]\cos(\Psi) \tag{30}$$

$$B_{22} = \Delta\eta\sqrt{\kappa}\text{sech}[\psi]\tanh[\psi]\sin(\Psi), \tag{31}$$

with

$$\Delta = \frac{\sqrt{D}}{\omega_h^2}\ ,\ \psi = \eta(z - z_o)\ ,\ \Psi = -\zeta z + \sigma. \tag{32}$$

We have used the conserved quantities norm $\mathcal{M}$ and momentum $\mathcal{P}$ of the envelope $F(z,t)$ to derive the evolution equations for the collective variables in the presence of the perturbation $R$. There also exist more pretentious perturbation methods which are based on the inverse scattering technique (IST) for the NLS [15], but the quality of the theory is mainly determined by the choice of the adiabatic ansatz (17) and not by the perturbation technique. More importantly, the employed perturbation theory yields simple stochastic equations where only the collective variables $\eta$ and $\zeta$ depend on the noise, which will be helpful in the calculations of the next section.

## 5 Langevin system

### 5.1 Derivation of the Langevin system

As the equations (26) can not be solved analytically, we try to find a mathematically less complicated but statistically equivalent system of stochastic equations for the CV. We derive the Fokker-Planck equation belonging to the system (26) and search for a system of Langevin equations which has the same Fokker-Planck equation. In this case the Langevin system and the system (26) are statistically equivalent. If we express the system (26) in the following compact nomenclature

$$\frac{dx_i}{d\tau} = A_i[\boldsymbol{x}] + \int_{-\infty}^{\infty} dz B_{ij}[z,\boldsymbol{x}]\xi^j(z,\tau), \tag{33}$$

the associated Fokker-Planck equation in Stratonovich interpretation reads

$$\partial_\tau\rho = -\sum_i^4 \partial_{x_i}\left[\rho A_i\right] + \frac{1}{2}\sum_{ijkm}^4 \int_{-\infty}^{\infty} dz \partial_{x_i}\left[B_{ij}\partial_{x_m}\left(\rho B_{mk}\right)\right]. \tag{34}$$

During the calculation of the Fokker-Planck equation we benefit from the fact that $\zeta(t)$ is restricted to small values such as $\sqrt{D} \sim \epsilon^3$ since $\zeta(t)$ lacks a drift term in (26) and starts at $\zeta(0) = 0$. Therefore we neglect the term $\zeta z$ in the trigonometric functions in (28–31) because $\sigma(t)$ is the dominating term. After calculating (34) one must derive formally the Fokker-Planck equation in Stratonovich interpretation for the Langevin system

$$\frac{dx_i}{d\tau} = a_i(\boldsymbol{x},\tau) + b_{ij}(\boldsymbol{x},\tau)\bar{\xi}^j(\tau) \tag{35}$$

$$\left\langle \bar{\xi}^i(t)\bar{\xi}^j(s) \right\rangle = \delta(t-s)\delta_{ij} \tag{36}$$

and determine the coefficients which result in the Fokker-Planck equation (34). The result of this procedure reads

$$\frac{d}{dt}\begin{pmatrix} \eta \\ \zeta \\ \sigma \\ z_o \end{pmatrix} = \begin{pmatrix} -\nu_{St}\eta \\ 0 \\ -\frac{\omega_h}{8}(\eta^2 - \zeta^2) \\ \frac{\omega_h}{4}\zeta \end{pmatrix} + \begin{pmatrix} b_{11} & 0 & 0 & 0 \\ 0 & b_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \bar{\xi}^1 \\ \bar{\xi}^2 \\ \bar{\xi}^3 \\ \bar{\xi}^4 \end{pmatrix}, \tag{37}$$

where

$$b_{11} = -\frac{\sqrt{3D\gamma}}{2\alpha}\sqrt{\eta}(\sin(\sigma) + \cos(\sigma)) \tag{38}$$

$$b_{22} = -\frac{\sqrt{D\gamma}}{2\alpha}\sqrt{\eta}(\cos(\sigma) + \sin(\sigma)). \tag{39}$$

At this point, we can compare our result with the Langevin set in [10] for the pulse solitons where we keep in mind that the situation is not identical because hydrodynamical damping was used in [10]. There are two important differences for the two soliton types. The amplitude of the pulse solitons decreases slower in time than for envelope solitons because of the damping. This fact is one reason why the observation of the soliton was possible for much longer times ($t \gg \frac{1}{\nu_{St}}$) in [10]. The diffusion of the pulse solitons is also stronger for small-amplitude solitons while the opposite is valid for envelope solitons due to the $\sqrt{\eta}$-term in $b_{22}$. If we substitute the ansatz for the envelope (17) in (9), the perturbed envelope soliton takes the form

$$\begin{aligned} y(z,t) &= Fe^{i\theta} + \tilde{F}e^{-i\theta} \\ &= 2\frac{\eta(t)}{\sqrt{\kappa}}\text{sech}\Big[\eta(t)(z - z_o)\Big] \\ &\quad \times \cos\left(kx - \zeta z - \omega_h t + \sigma\right). \end{aligned} \tag{40}$$

The two parameters $\zeta(t)$ and $z_o(t)$ with $\zeta(0) = z_o(0) = 0$ are only nonzero if we consider a noisy chain because $b_{22}$ is nonzero in this case. The component $\zeta z$ provides only small values with mean zero within the spatial extension of the envelope. The phase $\sigma(t)$ is a function of time because it is dependent both on $\eta(t)$ and on $\zeta(t)$ for $T > 0$, multiplied by $\omega_h$. This phase $\sigma(t)$ and the expression $\omega_h t$ result in a new time-dependent dispersion relation and therefore in a time-dependent velocity $v(t)$ of the wave packet. This relation is essential in order to calculate the velocity of the damped soliton where $\sigma(t)$ only depends on $\eta(t)$. We are interested in the diffusion of the soliton, thus $z_o(t)$ is the important quantity because it presents the spatial dislocations of the envelope due to the noise in the system. The damping also changes the soliton position via the variable $\sigma(t)$ but this mechanism is quasi-deterministic because $\sigma(t)$ only performs small fluctuations. Therefore the dislocation $z_o(t)$ essentially determines the soliton diffusion. The two parameters $\eta(t)$ and $\sigma(t)$ are dominated by the deterministic part of (37). We use this fact to derive an approximate analytical expression for $Var[z_o]$ in the next section. This analytical result is tested by the result for $Var[z_o]$ from the numerical solution of the set (37) where we have used 1000 runs with different random numbers. The analytical result for $Var[z_o]$ shows the correct dependence on the external parameters $\nu_{St}$, $T$, $c_o$ and the scaled time $\bar{t} = \nu_{St} t$.

### 5.2 Analytical approach

The drift term of $\eta(t)$ in (37) is responsible for the exponential decay of $\eta(t)$ which starts at $t = 0$ with $\eta_o \sim \epsilon$. The fluctuations of $\eta(t)$ are usually less than five percent after typical times $\bar{t} = \nu_{St} t \approx 2$. Therefore $\eta(t)$ and $\sigma(t)$ (which primarily depends on $\eta(t)$) can be replaced by the expressions of the damped system without noise

$$\eta(t) = \eta_o e^{-\nu_{St} t} \tag{41}$$

$$\sigma(t) = -\frac{(c_o^2 - 1) w_h}{4\nu} \left(1 - \exp(-2\nu_{St} t)\right). \tag{42}$$

This approximation means we have neglected the influence of the noise term $\bar{\xi}^1$ in our system. The remaining part of system (37) is

$$\frac{d}{dt}\begin{pmatrix} \zeta \\ z_o \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{\omega_h}{4}\zeta \end{pmatrix} + \begin{pmatrix} -C_1 e^{-\frac{\nu}{2}t}(\cos(\sigma) + \sin(\sigma)) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \bar{\xi}_1 \\ \bar{\xi}_2 \end{pmatrix}, \tag{43}$$

where

$$C_1^2 = \frac{D\gamma\sqrt{c_o^2 - 1}}{2\alpha^2} = \frac{\nu_{St} T \gamma \sqrt{c_o^2 - 1}}{\alpha^2}. \tag{44}$$

This system can be written as ($x_1 = \zeta$, $x_2 = z_o$)

$$\frac{dx_i}{dt} = -A_{ij}(t) x_j + B_{ij}(t) \bar{\xi}^j(t). \tag{45}$$

We find an analytic expressions for the quantities $Var[z_o] = \langle x_2^2 \rangle$ and $Var[\zeta] = \langle x_1^2 \rangle$ using the relation

$$\frac{d}{dt}\Big\langle x_i x_j \Big\rangle = -\mathbf{A}_{il}\Big\langle x_l x_j \Big\rangle - \Big\langle x_i x_l \Big\rangle (\mathbf{A}^T)_{lj} + \mathbf{D}_{ij} \tag{46}$$

[16] with

$$\mathbf{A} = \begin{pmatrix} 0 & 0 \\ -\frac{w_h}{4} & 0 \end{pmatrix} \tag{47}$$

$$\mathbf{B} = \begin{pmatrix} -C_1 e^{-\frac{\nu_{St}}{2}t} f[\sigma(t)] & 0 \\ 0 & 0 \end{pmatrix} \tag{48}$$

$$\mathbf{D} = \mathbf{B}\mathbf{B}^T = \begin{pmatrix} C_1^2 e^{-\nu_{St} t} f[\sigma(t)]^2 & 0 \\ 0 & 0 \end{pmatrix} \tag{49}$$

$$f[\sigma(t)] = \cos[\sigma(t)] + \sin[\sigma(t)]. \tag{50}$$

For $Var[z_o]$, the result reads

$$\begin{aligned} Var[z_o] &= \frac{C_2}{2}\int_0^t e^{-\nu t'} f[\sigma(t)]^2 (t - t')^2 dt' \\ &\approx C_2 \int_0^t e^{-\nu t'} (t - t')^2 dt' \\ &= K\left(1 - \exp(-\bar{t}) - \bar{t} + \frac{\bar{t}^2}{2}\right) \end{aligned} \tag{51}$$

with

$$C_2 = \frac{\omega_h^2}{8} C_1^2 \tag{52}$$

$$K = \frac{C_2}{\nu_{St}^3} = \frac{\omega_h^2 \sqrt{c_o^2 - 1}\,\gamma k_B T}{8\alpha^2 \nu_{St}^2}. \tag{53}$$

Already for small times $\bar{t}$ ($t \ll \nu_{St}^{-1}$) the diffusion is anomalous

$$Var[z_o] \cong K\left(\frac{\bar{t}^3}{3!} - \frac{\bar{t}^4}{4!} + ...\right). \tag{54}$$

The result is surprising since the pulse solitons show a normal diffusion behaviour for small times [10]. The superdiffusive term in the position variance of pulse solitons ($\sim t^2$) is negligibly small until several time units $\bar{t}$ have passed. The anomalous behaviour appears sooner the higher the velocity of the initial pulse is chosen. Our theory for the perturbed envelope soliton also predicts a dominance of the quadratic term for large times $\bar{t}$ ($t \gg \nu_{St}^{-1}$)

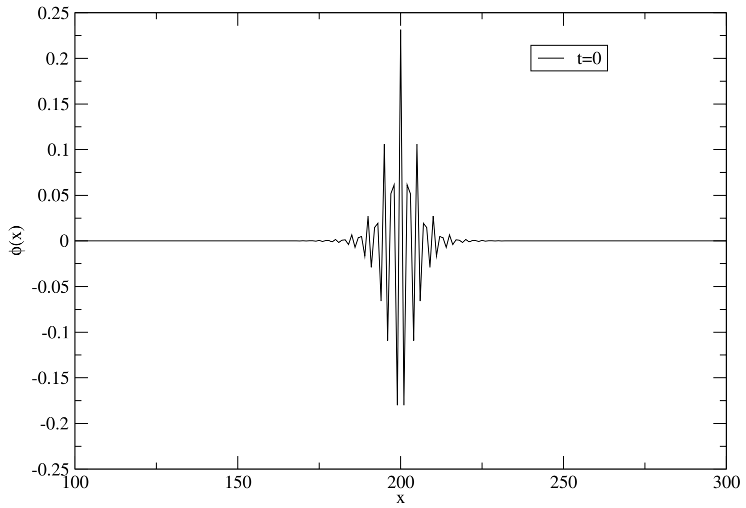
$$Var[z_o] \cong K\frac{\bar{t}^2}{2}, \tag{55}$$

although in the simulations, it was not possible to investigate the diffusion of the envelope solitons for similar large times as it was done for the pulse solitons.

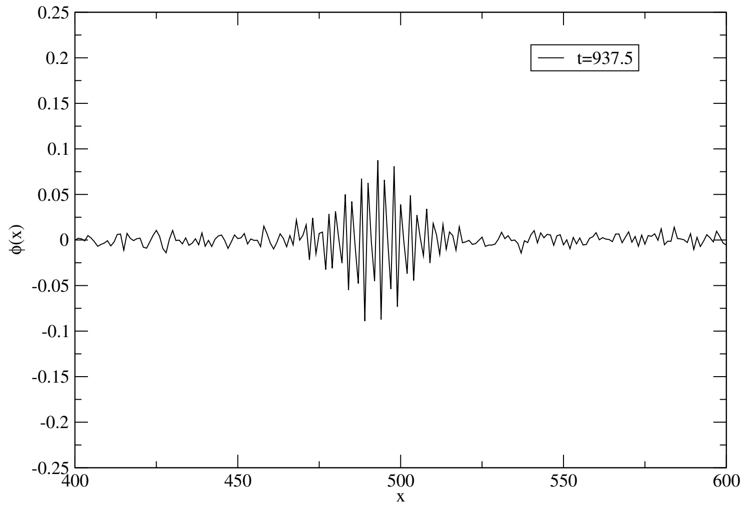
We compare the result (51) for $Var[z_o]$ with the simulations of an envelope soliton on a noisy and damped chain, namely the quantity $Var[x_s]$. We must check if the simulations show the predicted proportionalities

$$Var[x_s] \sim \frac{\sqrt{c_o^2 - 1}}{\nu_{St}^2} T \tag{56}$$

and the time dependence of $Var[z_o]$.




(a) $t = 0$




(b) $t = 937.5$

**Fig. 1.** Envelope soliton ($k = \frac{4\pi}{5}$, $c_o = 1.01$) on a damped ($\nu_{St} = 0.001$) and noisy chain ($T = 5 \times 10^{-5}$).

Before we compare the theoretical result $Var[z_o]$ with the values $Var[x_s]$ from the simulations, we should recapitulate the numerical methods we applied.

## 6 Simulations

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

$$\ddot{\phi}_n = \alpha[\phi_{n+1} - 2\phi_n + \phi_{n-1}] + \gamma[\phi_{n+1}^3 - 2\phi_n^3 + \phi_{n-1}^3] - \nu_{St}\dot{\phi}_n + \sqrt{D}(\xi_{n+1}(t) - \xi_n(t)), \quad (57)$$

where we always choose $\alpha = \gamma = 1$ in the simulations. We use periodic boundary conditions in order to be able to run long simulation times

$$\frac{d^l\phi_0}{dt^l} = \frac{d^l\phi_{N-1}}{dt^l}, \quad \frac{d^l\phi_N}{dt^l} = \frac{d^l\phi_1}{dt^l}, \quad l = 0, 1$$
$$\xi_0(t) = \xi_{N-1}(t), \quad \xi_N(t) = \xi_1(t). \quad (58)$$

The simulations are performed on a chain with at least 1000 lattice points. The time integration is carried out by using the Heun method [17] which has been successfully used in the numerical solution of partial differential equations and difference-differential equations, coupled to either an additive or a multiplicative noise term [11,18–20]. At $t = 0$ the chain is initialized by a discrete version of the envelope soliton (15). In Figure 1 one can see the initial condition at $t = 0$ and a snapshot of the chain at a later time t comparable with $\bar{t} = 1$. The envelope soliton decreases due to the damping. The particles on the chain show appreciable fluctuations from their positions due to the temperature although we chose very small values for $\nu_{St}$ and $T$. We detect the position of the envelope soliton $x_s$ for 50 realizations and calculate the variance of the soliton position $Var[x_s]$. We use relative coordinates because in this representation the amplitude of the envelope soliton vanishes at infinity. In order to detect the center of the soliton we search for the center of the norm $M$ of

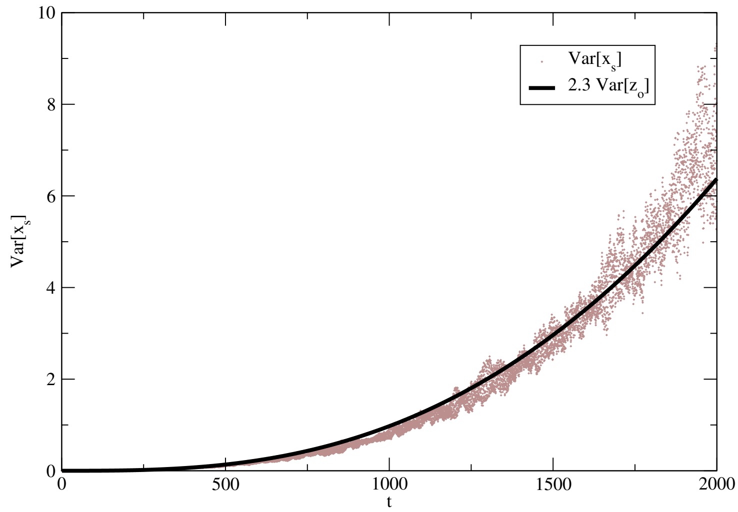



**Fig. 2.** The scaled ($c = 2.3$) solution $Var[z_o]$ agrees with the result $Var[x_s]$ of the simulation ($c_o = 1.01$, $\nu_{St} = 0.001$, $T = 5 \times 10^{-5}$).

the envelope soliton. The norm $M$ is a conserved quantity for the unperturbed soliton because it is twice the norm $\mathcal{M}$ of the envelope in the continuum limit

$$M = \int_{-\infty}^{\infty} \phi(x,t)^2 dx \overset{(9)}{\approx} 2 \int_{-\infty}^{\infty} \mid G(x,t) \mid^2 dx \qquad (59)$$
$$= 4 \frac{\sqrt{c_o^2 - 1}}{\kappa_r} = M_o.$$

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 $M$

$$x_s(t) = \frac{\sum_{i=n_1}^{n_2} i\phi_i^2}{\sum_{i=n_1}^{n_2} \phi_i^2}, \qquad (60)$$

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. For the damped system, the norm of the envelope soliton $M_o$ decays exponentially ($\sim e^{-2\Gamma\tau} = e^{-\nu_{St} t}$). After several units of $\bar{t}$ the amplitude of the envelope soliton (in relative coordinates) becomes comparably small with the thermal fluctuations of the particles and the position routine then fails. This failure is the reason why we are not able to investigate the diffusive behaviour of the envelope soliton for similar long times $t \gg \frac{1}{\nu_{St}}$ as it was done for pulse solitons in [10]. Larger values of $\eta_o$ would be helpful yet we are restricted to small values $\mathcal{O}(\epsilon)$ due to the CA. 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. In comparison, the particles in the profile of a pulse soliton move much slower and therefore dissipate less energy.

## 7 Discussion

We compare the results from the simulations with the analytical expression (51) in the following figures. We present the soliton diffusion $Var[x_s]$ for two envelope solitons differentiated by their velocities $c_o = 1.01$ (Fig. 3) and $c_o = 1.03$ (Fig. 4) with varying damping $\nu_{St}$ and temperature $T$. The solid line in Figures 3 and 4 presents the analytical result $Var[z_o]$ for the position variance $Var[x_s]$ according to (51). We only present the results for times $\bar{t} \leq 2$ since for small velocities $c_o$ the damped envelope solitons become strongly masked by noise and the position routine begins to fail for $\bar{t} > 2$. The values of the simulation results are always larger than the theoretical prediction $Var[z_o]$, where the difference depends on the choice of the parameters $\nu_{St}$, $T$ and the normalized velocity $c_o$. This fact is expected since we only considered the influence of the noise on the soliton. The contribution of the phonons to the diffusion of the envelope soliton is not taken into account in our calculations. One knows from different systems that the soliton-phonon scattering also contributes to the soliton diffusion. It was recently shown by simulations of anharmonic atomic chains that the phonon bath yields a significant contribution (linear in time) to the diffusion of pulse solitons with velocities close to the sound velocity [10]. The soliton shift caused by the scattering was analytically calculated only in the integrable Toda lattice [21]. The result allows the determination of the phonon contribution to the diffusion of the pulse solitons and it can be shown that the phonons cause an additional normal diffusion term which depends quadratically on the temperature of the phonon bath [22]. Although we could not consider this additional effect in the case of the envelope solitons, the time dependence of $Var[z_o]$ and $Var[x_s]$ is always very similar. If one scales $Var[z_o]$ for a certain parameter set $(c_o, \nu_{St}, T)$ with a constant factor $c > 1$, one always obtains a good agreement with the theory (Fig. 2). This agreement seems to be typical

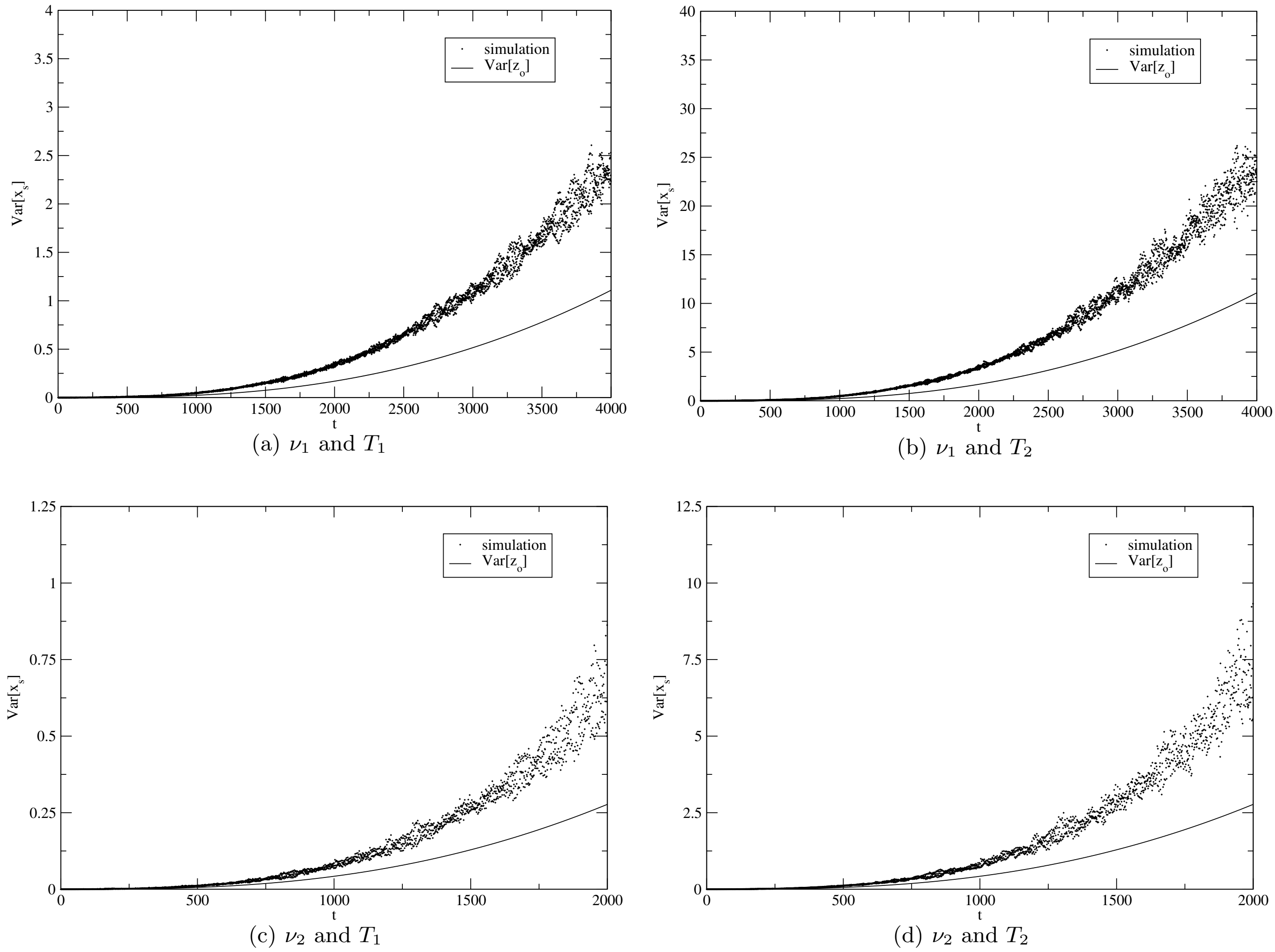



**Fig. 3.** $Var[x_s]$ for an envelope soliton with $c_o = 1.01$: simulation vs. result (49). ($\nu_1 = 0.0005$, $\nu_2 = 0.001$, $T_1 = 5 \times 10^{-6}$, $T_2 = 5 \times 10^{-5}$).

for the diffusion of nonlinear excitations since such differences also occur with the pulse solitons on the anharmonic chain or with vortices in the 2D Heisenberg model [10,18]. The predicted linear dependence of $K$ in (54) on temperature $T$ reflects the simulation results precisely. If the temperature $T_1 = 5 \times 10^{-6}$ in Figures 3 and 4 is replaced by $T_2 = 5 \times 10^{-5}$, then the values of $Var[x_s]$ increase by a factor of 10. The proportionality $Var[z_o] \sim \frac{1}{\nu^2}$ is also confirmed by the simulation results for small values of the normalized velocity ($c_o < 1.03$). The $c_o$-dependence of $Var[z_o]$ concurs only qualitatively with the simulations. According to the factor $\sqrt{c_o^2 - 1}$, the values for the soliton diffusion in (a), (b), (c) and (d) in Figure 4 for the soliton with $c_o = 1.03$ should be approximately 1.74 times larger than the values in Figure 3 for the soliton with $c_o = 1.01$. Yet the observed values for the diffusion grow slower than the factor $\sqrt{c_o^2 - 1} = \frac{\eta_o}{2}$ indicates, which represents the amplitude or the inverse width of the initial soliton. Such differences can be expected, since it is known that the adiabatic approach bears certain problems especially when one predicts the shape of a perturbed envelope soliton for large times. The perturbation normally destroys the coupling between amplitude and inverse width of the unperturbed soliton. It is also of note that the underlying perturbation theory is based both on an NLS-type equation and on the bright soliton solution which are only good approximations for small $c_o$ and small perturbations.

Nevertheless, the adiabatic perturbation theory is capable of explaining the most important results of the simulations. The envelope solitons exhibit a superdiffusive behaviour like pulse solitons yet they show a very different time dependence, especially concerning small times. The expression (51) explains why the short-time behaviour is dominated by anomalous diffusion terms and how the position variance grows with increasing velocities $c_o$. In the case of pulse solitons $Var[x_s]$ decreases with increasing $c_o$ since in this case the linear diffusion term decreases. The superdiffusive quadratic term begins to dominate after longer times. Our simulations and theory prove that the perturbed envelope and pulse solitons behave very

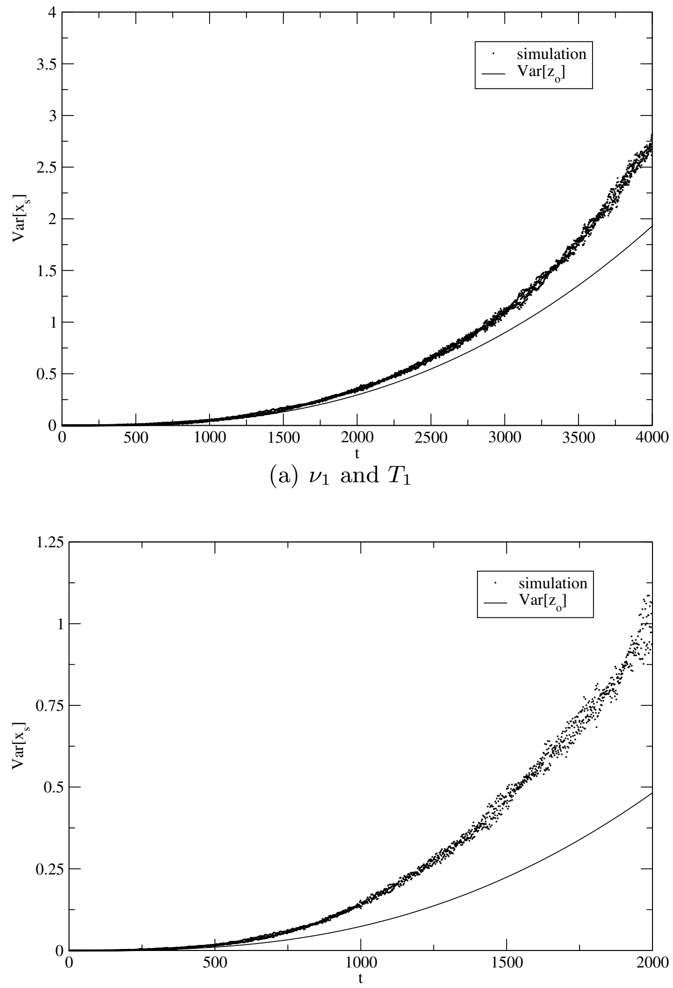



**Fig. 4.** $Var[x_s]$ for an envelope soliton with $c_o = 1.03$: simulation vs. result (49). ($\nu_1 = 0.0005$, $\nu_2 = 0.001$, $T_1 = 5 \times 10^{-6}$, $T_2 = 5 \times 10^{-5}$).

differently although they are both non-topological solitons in contrast to topological solitons which do not show superdiffusion.

The pulse solitons show a normal diffusion for small times due to the noisy dynamics of the soliton center. The anomalous diffusion, which stems from the fluctuations of the soliton width, becomes dominat for larger times. We have shown that the envelope solitons reveal a different diffusion mechanism. The damping causes a rapidly growing width of the envelope. The envelope solitons appear much more like non-rigid objects than the pulse solitons. This effect leads to the anomalous diffusion of the envelope solitons for all times.

We want to thank Edward Arévalo (MPI PKS Dresden) for various discussions concerning the simulations of the discrete chain and Chris Tarn (University Bayreuth) for the critical reading of this manuscript.

## References

1. N.J. Zabusky, M.D. Kruskal, Phys. Rev. Lett. **15**, 240 (1965)
2. P. Perez, N. Theodorakopoulos, Phys. Lett. A **117**, 405 (1986)
3. D. Hochstrasser, F.G. Mertens, H. Büttner, Phys. Rev. A **40**, 2602 (1989)
4. S. Yomosa, Phys. Rev. A **32**, 1752 (1985)
5. P. Perez, N. Theodorakopoulos, Phys. Lett. A **124**, 267 (1987)
6. M. Wadati, J. Phys. Soc. Jpn **38**, 673 (1976)
7. M. Peyrard, A.R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989)
8. T. Dauxois, M. Peyrard, A.R. Bishop, Phys. Rev. E **47**, 684 (1993)
9. N. Flytzanis, S. Pnevmatikos, M. Remoissenet, J. Phys. C **18**, 4603 (1985)
10. E. Arévalo, F.G. Mertens, Y. Gaididei, A.R. Bishop, Phys. Rev. E **67**, 016610 (2003)
11. M. Meister, F.G. Mertens, A. Sánchez, Eur. Phys. J. B **20**, 405 (2001)
12. A. Tsurui, Prog. Theor. Phys. **48**, 1196 (1972)

13. E. Arévalo, Y. Gaididei, F.G. Mertens, Eur. Phys. J. B 27, 63 (2002)
14. V. Konotop, L. Vázquez, *Nonlinear Random Waves* (World Scientific, Singapore, 1994)
15. F. Abdullaev, *Theory of Solitons in inhomogeneous Media* (John Wiley and Sons, New York, 1994)
16. J. Honerkamp, *Stochastische Dynamische Systeme* (VCH, Weinheim, 1990)
17. P. Kloeden, E. Platen, *Numerical solution of Stochastic Differential Equations* (Springer-Verlag, 1992)
18. T. Kamppeter, F.G. Mertens, E. Moro, A. Sanchez, A.R. Bishop, Phys. Rev. B **59**, 11349 (1999)
19. M. Meister, F.G. Mertens, J. Phys. A **33**, 2195 (2000)
20. N. Quintero, A. Sánchez, F.G. Mertens, Eur. Phys. J. B **16**, 361 (2000)
21. N. Theodorakopoulos, F.G. Mertens, Phys. Rev. B **28**, 3512 (1983)
22. F.G. Mertens, E. Arévalo, A.R. Bishop, submitted to Phys. Rev. E