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EFFECTS OF NOISE ON LOCALIZED EXCITATIONS IN THE DISCRETE NONLINEAR SCHRÖDINGER SYSTEM

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Abstract. In the framework of the discrete nonlinear Schrödinger equation with nearest-neighbour coupling we discuss the stability of highly localized, "breather-like" excitations under the influence of thermal fluctuations. Numerical analysis shows that the lifetime of the breather is always finite and in a large parameter region inversely proportional to the noise variance for fixed damping and nonlinearity. We also find that the decay rate of the breather decreases with increasing nonlinearity and with increasing damping.

Key words: nonlinear Schrödinger equation, white noise, breathers.

The effects of noise on the localized excitations in the discrete nonlinear Schrödinger (DNLS) equation with only nearest-neighbour interaction is considered. The investigation is motivated by the need to understand the temperature effects in molecular systems. A frequently used method for taking into account effects of finite temperature in models describing a quantum quasi-particle (electron or exciton) interacting with lattice vibrations is to add white noise and damping to the lattice equations [1, 2], thereby turning these into Langevin equations. As shown in [1, 2], the coupled exciton-phonon equations can under certain approximations be reduced to a single DNLS equation describing the exciton dynamics, where the effects of thermal fluctuations of the phonons appear as a multiplicative noise term. The spectrum of the noise will then in general be coloured, but assuming short correlation times it can be treated as white noise in the first approximation. In order to take proper account of the damping of the phonon system, it is necessary (at least when the white noise approximation is made) to additionally include a nonlinear damping term in the exciton equation [1, 2]. With this inclusion, it was shown that energy balance may be established in the exciton system. On this background we consider in this paper the one-dimensional DNLS equation with multiplicative noise and nonlinear damping included, and investigate how these terms affect the discrete breathers.

The form of the DNLS equation considered here is the following:

$$i\dot{\psi}_n + J(\psi_{n+1} + \psi_{n-1}) + \gamma|\psi_n|^2\psi_n - \eta\psi_n\frac{d}{dt}(|\psi_n|^2) + h_n(t)\psi_n = 0, \tag{1}$$

where the last two terms describe nonlinear damping and multiplicative Gaussian white noise, respectively. The noise is assumed to have zero mean and variance $2D$, i.e.,

$$\langle h_n(t)\rangle = 0, \;\; \langle h_n(t)h'_n(t')\rangle = 2D\delta(t-t')\delta_{nn'}. \tag{2}$$

Equation (1) can be derived from the equation of motion for a quantum quasi-particle (e.g., electron or exciton) treated in the nearest-neighbour tight-binding approximation and interacting with a classically treated optical phonon field in contact with a heat bath, i.e. (in units of $\hbar = 1$),

$$i\dot{\psi}_n + J(\psi_{n+1} + \psi_{n-1}) + \chi u_n\psi_n \;=\; 0, \tag{3}$$

$$M\ddot{u}_n + M\lambda\dot{u}_n + M\omega_0^2 u_n - \chi|\psi_n|^2 \;=\; \sigma_n(t). \tag{4}$$

Here ψ_n is the amplitude of the quasi-particle wave function at site n and u_n represents the elastic degree of freedom at site n. Furthermore, J is the nearest-neighbour hopping constant, χ is the coupling constant between the quasi-particle and the phonons, M is the molecular mass, λ is a damping coefficient, ω_0 is the Einstein frequency of each oscillator, and $\sigma_n(t)$ is a stochastic force acting on the phonon system. Equation (4) is the Langevin equation for the phonon system, so the variance of the stochastic force is related to the external temperature T and the damping coefficient λ according to the fluctuation-dissipation theorem. The DNLS equation can be derived from Eqs. (3) and (4) if the quasi-particle field is assumed to vary slowly in time compared with the lattice vibrations [1, 2]. This results in the following relation between the parameters of Eqs. (1)–(4):

$$\gamma = \frac{\chi^2}{M\omega_0^2}, \;\; \eta = \gamma\frac{\lambda}{\omega_0^2}, \;\; D = \eta k_B T, \tag{5}$$

where k_B is the Boltzmann constant.

The DNLS equation has as its only conserved quantity the excitation number, $N = \sum_n |\psi_n|^2$, while the Hamiltonian H_{DNLS}

$$H_{\mathrm{DNLS}} = -J\sum_n\left(\psi_n\psi_{n+1}^* + \psi_n^*\psi_{n+1}\right) - \frac{\gamma}{2}\sum_n|\psi_n|^4, \tag{6}$$

will evolve according to

$$\frac{dH_{\text{DNLS}}}{dt} = -\eta \sum_n \left(\frac{d}{dt}(|\psi_n|^2) \right)^2 + \sum_n h_n(t) \frac{d}{dt} \left(|\psi_n|^2 \right) \tag{7}$$

indicating that the damping and noise terms on average provide dissipation and energy input, respectively.

We integrate Eq. (1) numerically using a single-site initial condition,

$$\psi_n(0) = \delta_{n,n_0}, \tag{8}$$

varying the parameters γ, η, and D for the fixed values $N = 1$ and $J = 1$, and using a lattice large enough to simulate an infinite chain. For this choice of initial condition the DNLS equation exhibits a self-trapping transition at $\gamma = \gamma_c \simeq 3.5$ when $\eta = D = 0$; when $\gamma > \gamma_c$, a finite part of the excitation will remain trapped around the initial site during the time evolution [3–5]. As γ is increased beyond γ_c, the total excitation number of the part trapped around the initial site increases, and the width of the excitation decreases. In the calculations reported here, we consider nonlinearities $\gamma \geq 5$, for which the trapped excitation has a highly discrete, breather-like nature.

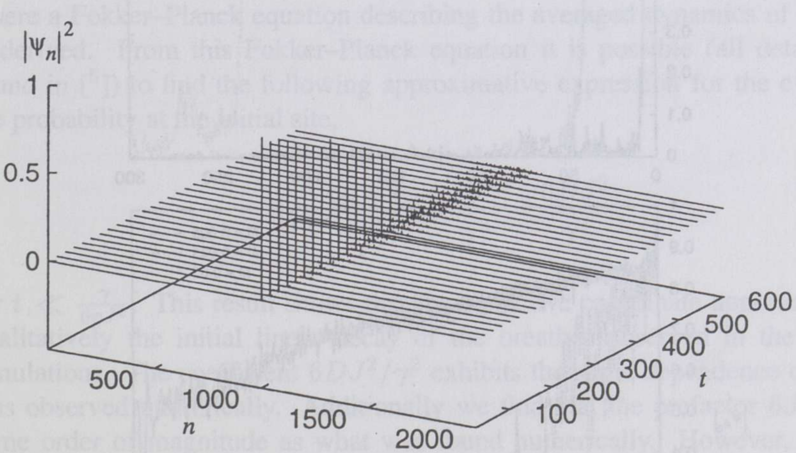

Fig. 1. Evolution of an initially single-sited localized excitation. Parameter values are $\gamma = 10$, $\eta = 2$, and $D = 0.05$.

An illustration of how the presence of noise in Eq. (1) affects the DNLS breathers is given in Figs. 1 and 2. We see that after a short initial interval, where the breather is created and the initial-site probability $|\psi_{n_0}|^2$ rapidly drops to a value close to its stationary value in the absence of noise, the noise will cause a slow, almost linear, decrease in the breather intensity with time. This linear decay continues until the value of $|\psi_{n_0}|^2$ has been reduced to approximately half its initial value, at which point the initial-site probability rapidly drops to values close to

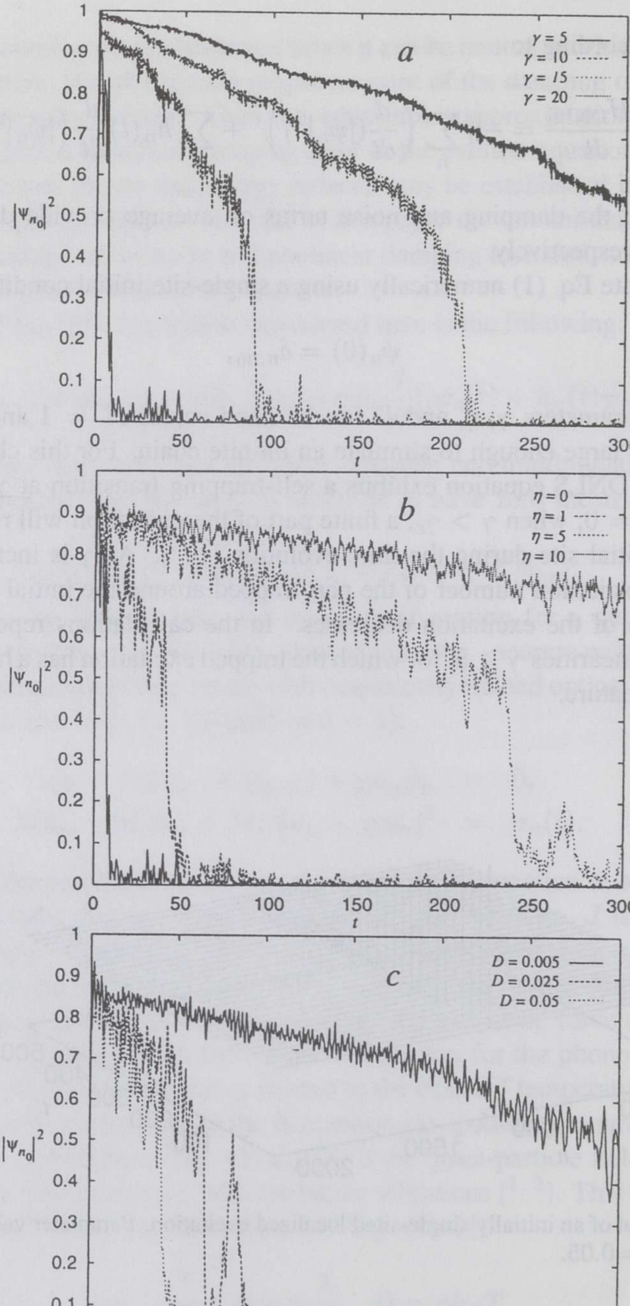

Fig. 2. Typical evolution of the initial-site probability for different values of γ, η, and D. In (a) we have $\eta = 0$, $D = 0.05$, and from bottom to top $\gamma = 5, 10, 15$, and 20; in (b) $\gamma = 5$, $D = 0.05$, and from bottom to top $\eta = 0, 1, 5$, and 10; in (c) $\gamma = 5$, $\eta = 1.0$, and $D = 0.005$, 0.025, and 0.05 from top to bottom. The particular realization of the noise is the same in all cases.

zero, signifying that the breather is destroyed. After this point the system behaves diffusively, similar to the corresponding linear system ($\eta = \gamma = 0$), with the initial-site probability decaying on average as $t^{-1/2}$. Thus, we find that the lifetime of the breather is always finite, but increases when (a) the nonlinearity γ is increased, (b) the nonlinear damping η is increased, or (c) the noise variance D is decreased (see Fig. 2). The quantitative influence of the parameters γ, η, and D on the lifetime has been investigated by performing numerical calculations for several different realizations of the noise, and determining the decay rate, κ, as the mean-value of $-\frac{d}{dt}\left(|\psi_{n_0}|^2\right)$ in the time interval of almost linear decay. Some of these results are displayed in Fig. 3. Figure 3a indicates that the decay rate is proportional to the variance of the noise over a large parameter region. We found this proportionality to be valid as long as the noise is so weak that the creation of the breather is unaffected (if the noise is too strong, no breather-like state will be created, and the diffusive spreading starts immediately). As is shown in Fig. 3b, the decay rate for fixed D and η is approximately proportional to γ^{-2} in the studied parameter range, while the data in Fig. 3c, showing the variation of κ with η, do not seem to follow any simple scaling law.

In order to gain some analytical understanding of the effects imposed on the DNLS breathers by the presence of noise and nonlinear damping, we use a method of collective coordinates. This approach necessitates a rather elaborate analysis where a Fokker–Planck equation describing the averaged dynamics of the system is derived. From this Fokker–Planck equation it is possible (all details can be found in [6]) to find the following approximative expression for the evolution of the probability at the initial site,

$$\langle|\psi_{n_0}|^2\rangle \simeq 1 - \frac{2J^2}{\gamma^2} - \frac{6DJ^2}{\gamma^2}t \qquad (9)$$

for $t \ll \frac{\gamma}{6\eta J^2}$. This result shows that the collective coordinate approach explains qualitatively the initial linear decay of the breather observed in the numerical simulations. The coefficient $6DJ^2/\gamma^2$ exhibits the same dependence of D/γ^2 as was observed numerically. Additionally we find that the prefactor $6J^2$ is of the same order of magnitude as what was found numerically. However, due to the approximate character of the analytical approach, the η-dependence predicted by Eq. (9) differs from the numerical results.

In summary, we have found that introducing multiplicative white noise and nonlinear damping into the DNLS equation with nearest-neighbour coupling will cause decay of the self-trapped discrete breathers which are created for large nonlinearities. Numerical analysis showed that the intensity at the central breather-site would initially decrease approximately linearly with time. The decay rate was found to decrease with increasing nonlinearity γ and with increasing damping η, and to increase with increasing noise variance D.

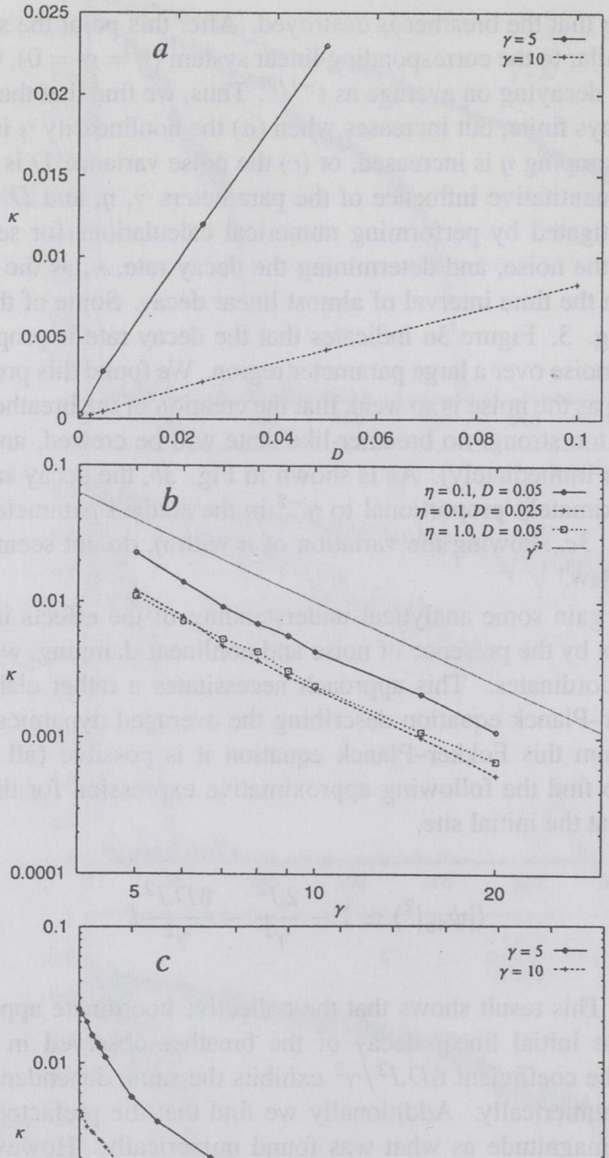

Fig. 3. Quantitative dependence of the decay rate, κ, of the breather as a function of (a) noise strength D, (b) nonlinearity parameter γ, and (c) nonlinear damping parameter η. In (a) $\eta = 0.1$ for both curves and in (c) $D = 0.05$ for both curves; other parameter values are as indicated in the figures.

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MÜRAEFEKTID LOKAALSELT HÄIRITUD DISKREETSES MITTELINEAARSES SCHRÖDINGERI SÜSTEEMIS

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Diskreetse mittelineaarse Schrödingeri võrrandi baasil on analüüsitud tugevasti lokaliseeritud briiseri tüüpi häirituste stabiilsust termiliste fluktuatsioonide korral. Mudel arvestab interaktsiooni ainult lähimate naabrite vahel. Numbriline analüüs näitas, et briiseri eluiga on alati lõplik ning pöördvõrdeline müra karakteristikuga fikseeritud sumbuvuse ja mittelineaarsuse korral.