Slow Relaxation Phenomena Induced by Breathers in Nonlinear Lattices

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We study relaxation properties of one dimensional nonlinear lattices which are initially thermalized and subsequently put intp contact with a cold bath simulated by absorbing boundary conditions. We observe a nonexponential lattice energy relaxation in contrast to the standard exponential relaxation law of the corresponding linear system. We connect the long-tail relaxation behavior with the presence of long-lived nonlinear localized modes. The mobility of the breathers is shown to play a substantial role in the lattice relaxation properties. [S0031-9007(96)01862-5]

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It is well known that glass and spin-glass materials exhibit nonexponential slow relaxation properties [1]. Such behavior is usually considered the consequence of a complex hierarchy of local minima in the energy of the system. These metastable states trap in their neighborhood the configuration of the system for very long times, leading to a slowing down of its dynamics. The aim of this Letter is to present numerical results related to extended nonlinear dynamical systems that were obtained with a simple method borrowed from the standard techniques for studying glasses. It is shown for the first time that there exist certain dynamical systems which, even though they do not exhibit any metastable states at all, nevertheless exhibit unambiguously slow relaxation behavior similar to those of glasses. In our numerical experiments, the slowing down of the dynamics is due to the spontaneous formation of dynamical structures which persist for long times and play the same role as the metastable states in glasses. These dynamical structures were found to consist of random distributions of pinned or weakly mobile breathers [2–10].

The existence of breathers, i.e., localized nonlinear periodic oscillations in extended discrete nonlinear systems, is well established [5]. Breather solutions have been proved to be linearly stable and robust under small perturbations in a wide class of nonlinear models [9]. They might be rather mobile or strongly pinned to the lattice depending on the specific model and its parameters. When they exist, these nonlinear localized modes show up spontaneously in the dynamics of nonlinear systems and may change substantially system characteristics, especially in regard to their thermal properties. In such nonlinear systems at finite temperature, a breather can act as a localized *hot spot,* i.e., a local accumulation of energy, which might be pinned in the lattice or may travel through it. When several pinned breathers exist in the system, part of its energy is trapped for a long time at these hot spots even though some energy exchange between breathers is possible through phase fluctuations. The lower the density of breathers, the weaker the rate of energy transfer will be. This should be contrasted with the corresponding situation in linear systems where only phonons contribute to the energy transfer. In that case local energy accumulation spontaneously generated by thermal fluctuations relaxes shortly, independently of amplitude.

The thermal shock numerical experiments we performed on several nonlinear models, chosen for having different breather properties, are motivated by analogous but real experiments (Refs. [11–13]) performed on real glassy systems. We considered one dimensional chains of anharmonic oscillators with free ends and also, for comparison, the harmonic systems which are equivalent at low temperature. The isolated system is put initially in a state at a given temperature T. Subsequently, at time zero, our system is put into contact with a bath at zero temperature and spontaneously commences relaxation towards its ground state. In our numerical experiments a number of end oscillators of the chain are submitted to an additional damping force and thus act as a heat sink for the thermal energy accumulated in the chain. We observe the relaxation rate of the total energy of the system.

The Hamiltonian of our one dimensional chain of N oscillators has the form

$$H = \sum_{n=1}^{N} \left[\frac{1}{2}\dot{u}_n^2 + W(u_{n+1} - u_n) + V(u_n) \right], \qquad (1)$$

where u_n is the dimensionless displacement of the nth oscillator from equilibrium, $\dot{u}_n$ its velocity. $W(u)$ is the nearest-neighbor coupling potential which is for most examples tested here, $W(u) = \frac{k}{2}u^2$. The constant k measures the strength of this coupling. $V(u)$ is a nonlinear on-site oscillator potential. We tested (i) the "hard" ϕ^4 potential $V(u_n) = \frac{1}{2}u_n^2 + \frac{1}{4}u_n^4$ and (ii) the "soft" Morse potential $V(u_n) = \frac{1}{2}[1 - \exp(-u_n)]^2$.

Both cases are approximate by the same harmonic potential $V(u_n) = \frac{1}{2}u_n^2$ at low temperature.

The lattices are originally brought into contact with a heat bath at temperature T (in units of lattice energy; Boltzmann's constant is taken equal to unity), for example, through the Nose method [14]. After the thermalization procedure is over we turn off the connection with the bath at temperature T and bring the lattice into contact with a zero temperature bath by adding damping to the system edge atoms.

Being in a nonequilibrium state the lattice evolves towards equilibrium through the equations of motion:

$$\ddot{u}_n = k(u_{n+1} - 2u_n + u_{n-1}) - V'(u_n) - \gamma \dot{u}_n(\delta_{n,L} + \delta_{n,R}), \quad (2)$$

where L and R denote all left-end and right-end contact oscillators, respectively, and δ denotes the Kronecker delta.

In Figs. 1 and 2 we present the basic results of our numerical study for the nonlinear potential of case (i). In Fig. 1 we show the spatiotemporal energy landscape of the lattice by plotting the local energy density in each lattice site and follow the thermalization process in time. The local energy density is the symmetrized total energy in each lattice site. In Fig. 2 we plot the normalized total lattice energy as a function of time for the temperature cases portrayed in Fig. 1 and also compare with the corresponding linear system. In Fig. 1 dark regions correspond to large local energy accumulation, whereas white regions designate low energy density. The case of temperature $T = 1$ corresponds to high energy for our energy scale. We note the clear presence of essentially pinned long-lived breathers that block the energy propagation towards the system edges. We also observe some

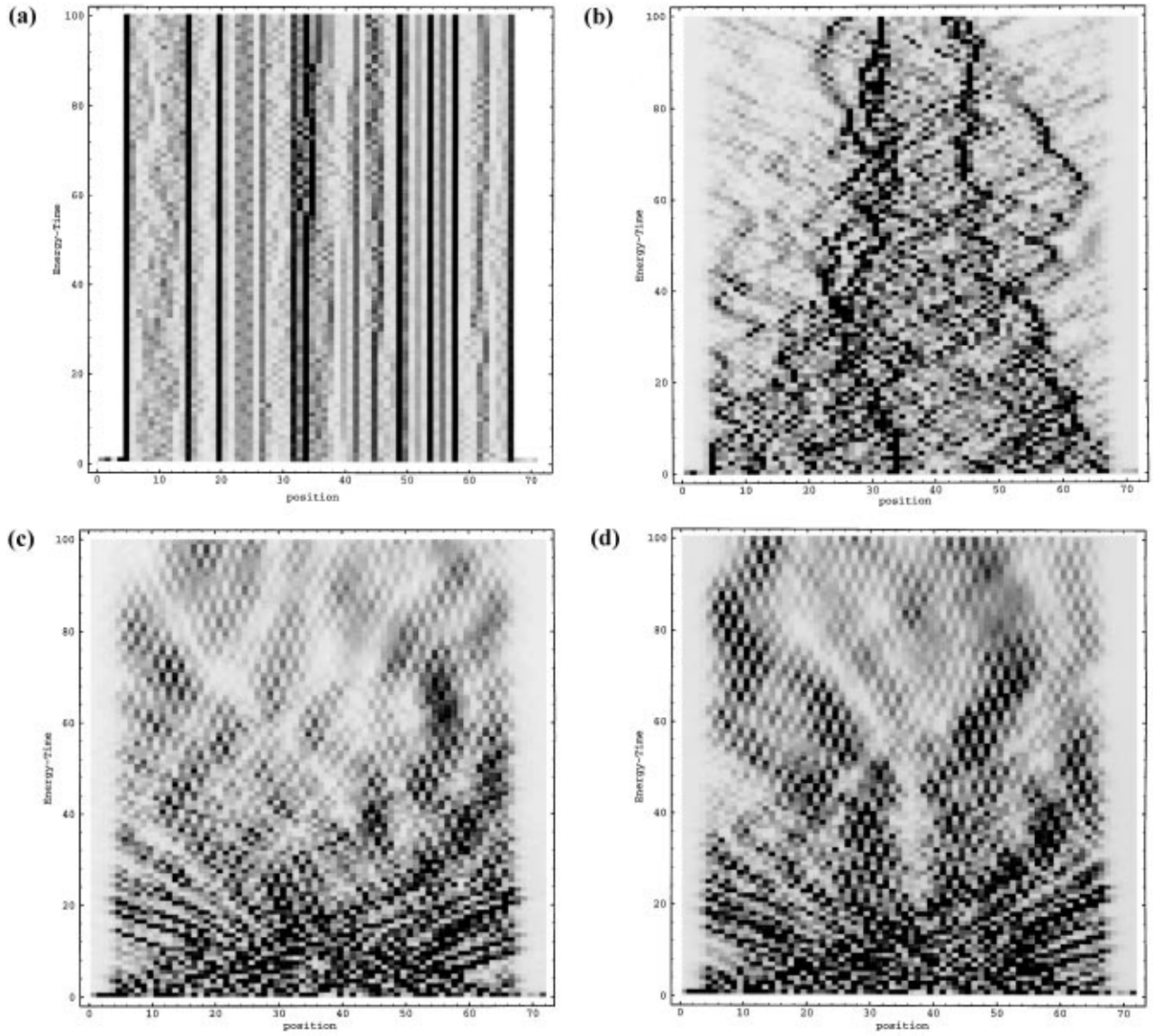

FIG. 1. Energy density landscape of a system of 72 particles as a function of time. Dark regions correspond to highs in local energy accumulation. In the horizontal axis we have the lattice sites whereas in the vertical local energy density snapshots of the entire system as a function of time. The lattices have been initially thermalized to (a) $T = 1$, (b) $T = 0.1$, (c) $T = 0.01$, (d) linear. The value of the coupling constant is $k = 0.1$, and damping of the edge atoms equals $\gamma = 0.1$.

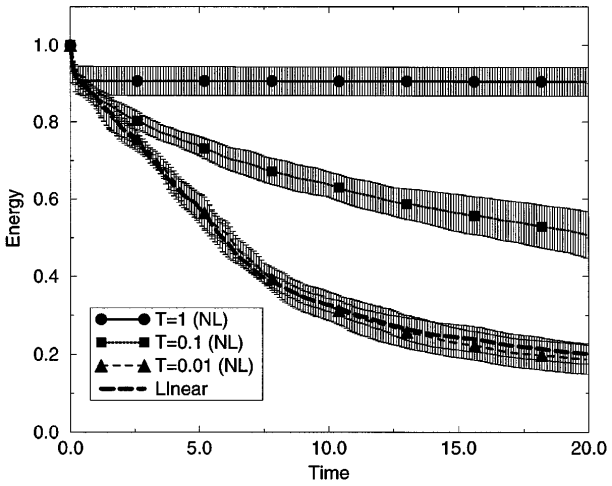

FIG. 2. Normalized averaged lattice energy decay as a function of time for the nonlinear ϕ^4 lattice (NL) with $A = B = 1$ and comparison with the corresponding linear lattice (L) with $A = 1$, $B = 0$. In all cases we use $k = 0.1$ and take 64 oscillators with eight additional bath oscillators, four on each end of the chain. The unit of time is equal to 100 periods of the linearized oscillators. The vertical lines are error bars over ten realizations. Both linear and nonlinear lattices were thermalized initially to $T = 1, 0.1, 0.01$, respectively. In the linear cases the relaxation rate is independent of the temperature.

creation and annihilation of localized modes. The breather structures seem to be opaque to local phonon mode propagation and as a result the system is completely partitioned in thermal cells. The macroscopic manifestation of this microscopic energy picture is clearly seen in the corresponding energy relaxation curve of Fig. 2. In the latter we observe an effective absence of relaxation after an initial small decay. When the system is thermalized to smaller temperatures [Fig. 1(b)] the breather content is lower while the breathers are now mobile. Because of breather creation and annihilation there is more de-trapping of energy, and as a result the energy decay of the system is faster (Fig. 2). We note that energy relaxation is still distinctly nonexponential and much slower than the exponential relaxation of the corresponding linear system also shown in Fig. 2 for comparison. In this intermediate regime, breather mobility contributes to the thermal relaxation properties of the lattice.

When the system temperature is reduced further, the breather size increases, and they quickly disappear from the picture; the energy relaxation is now completely phonon dominated since at small temperatures only the linear part of the potential is effective and thus energy relaxation proceeds in the usual exponential fashion (Fig. 2). We note that similar results were obtained for the homogeneously nonlinear case of the potential $V(u) = \frac{1}{4}u^4$ with the exception being that at small temperatures, due to the absence of phonon modes in this system, energy exchange is dominated by breathers diverging in size [15].

Having tested the case of the hard ϕ^4 potential we now turn to the soft Morse potential. The two nonlinear on-site potentials result in quite different breather properties at zero temperature. While in the hard ϕ^4 potential moving breathers were not identified at zero temperature, in the case of the Morse potential they do exist. Furthermore, Morse breathers exist below the phonon band that starts at the frequency of the linearized potential, viz., at frequency one, and extends to $\sqrt{1 + 4k}$. Before a sideband of a breather of frequency ω_b enters in the linear phonon spectrum the breather becomes unstable and decays [10]. An approximate maximal coupling where this instability that separates stable from unstable breathers occurs when

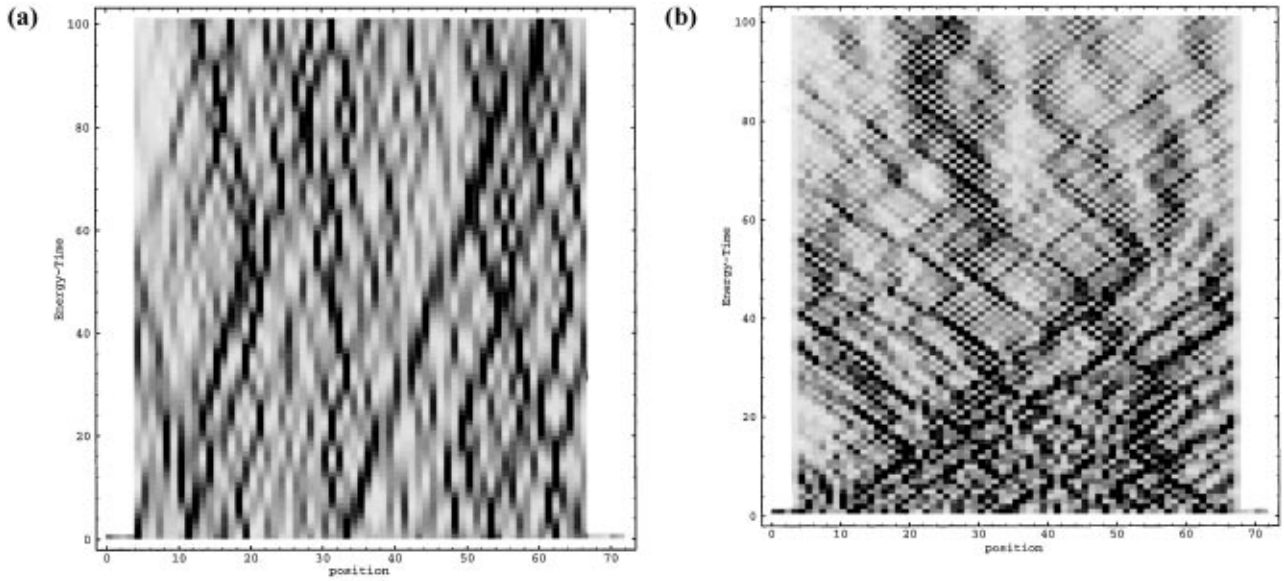

FIG. 3. Energy relaxation in a Morse chain of 72 particles as a function of time. We plot the local energy as function of time for a chain thermalized initially at $T = 0.001$. The dark regions correspond to local energy accumulation in (a) $k = 0.01$, (b) $k = 0.05$.

$\sqrt{1 + 4k_c} = 2$, viz., at $k_c = 3/4$. As a result we expect that *to the extent that breathers are responsible for energy relaxation in nonlinear systems* there will be a drastically different pattern in the equilibration for coupling values much smaller than the ones in the vicinity k_c. In Fig. 3 we show the "microscopic" flows of energy redistribution and relaxation for the Morse lattice at temperature $T = 0.001$ and two coupling constants k.

The energy landscape picture shows the existence of various regimes. At small coupling ($k = 0.01$) robust breathers are formed that are relatively immobile, but certainly much more mobile that the ones of the hard ϕ^4 potential lattice. At larger coupling ($k = 0.05$) the breathers become quite mobile, while at even further larger coupling they quickly diverge in size and thus assist in incoherent thermalization [15]. This microscopic picture is manifested in the macroscopic energy relaxation shown in Fig. 4. We note the clear nonexponential nature of the relaxation in the small and intermediate coupling regimes while there is an exact exponential relaxation curve in the high coupling regime. Near the coupling value $k = 0.4$ the Morse breather changes stability properties and becomes an unstable breatherlike extended phonon mode [10].

Although the system we studied has only one degree of freedom per unit cell, the existence of stable breathers is not subjected to this condition since we know that they can persist very generally in systems at any dimension and with many degrees of freedom per unit cell including acoustic phonons. The discrete breather induced phenomena of slow nonexponential relaxation that are shown here to be generic to discrete nonlinear lattice systems should also have distinct signatures in observables other than the energy distribution relaxation tail. They are expected to appear in equilibrium dynamical correlation functions evaluated at long times through long molecular dynamics simulations [16]. Furthermore, the effect of breathers in thermal system properties can be accentuated through the systematic introduction of spatially distributed thermal gratings. In this case we could partition the system into well separated, long-lived thermal cells that could be probed experimentally [15]. The glassy nature of extended discrete nonlinear systems found here could be connected to the well known slow thermalization properties of the Fermi-Pasta-Ulam model. Finally, it is possible that localized breather modes play also some role in the real glassy systems, an implication that is currently under investigation.

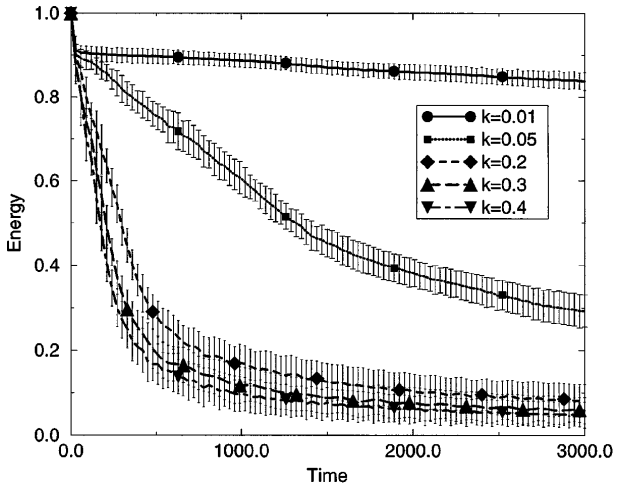

FIG. 4. Normalized averaged lattice energy decay as a function of time for the Morse lattice. We consider an initial thermalized state at $T = 0.001$ and vary the nearest-neighbor coupling k. The unit of time is equal to one oscillation period of the linearized local potential. The vertical lines are error bars over ten realizations. The distinctly nonexponential approach to equilibrium followed by long-lived saturation effects at small couplings are evident.

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[1] *Phase Transitions and Relaxations in Systems with Competing Energy Scales,* edited by T. Riste and D. Sherrington (Kluwer Academic, Dordrecht, 1993).
[2] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[3] D. K. Campbell and M. Peyrard, in *CHAOS—Soviet American Perspectives on Nonlinear Science,* edited by D. K. Campbell (American Institute of Physics, New York, 1990).
[4] S. Takeno and K. Hori, J. Phys. Soc. Jpn. **60**, 947 (1991).
[5] R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[6] K. S. Rasmussen, D. Hennig, G. P. Tsironis, and H. Gabriel, Phys. Rev. E **52**, 4628 (1995).
[7] D. Cai, A. R. Bishop, and N. Gronbech-Jensen, Phys. Rev. E **52**, 5784 (1995).
[8] S. Takeno and M. Peyrard, Physica (Amsterdam) **92D**, 140 (1996).
[9] S. Aubry, Physica (Amsterdam) D (to be published).
[10] J. L. Marin and S. Aubry, Nonlinearity (to be published).
[11] J. Zimmermann and G. Weber, Phys. Rev. Lett. **46**, 661 (1981).
[12] Yu. N. Ovchinnikov, K. Biljakovic, J. C. Lasjaunias, and P. Monceau, Europhys. Lett. **34**, 645 (1996).
[13] J. C. Lasjaunias, K. Biljakovic, and P. Monceau, Phys. Rev. B **53**, 7699 (1996).
[14] S. Nose, J. Chem. Phys. **81**, 551 (1984); Mol. Phys. **52**, 255 (1994).
[15] G. P. Tsironis and S. Aubry (to be published).
[16] S. Flach and G. Mutschke, Phys. Rev. E **49**, 5018 (1994).