BRIEF REPORTS

Brief Reports are accounts of completed research which do not warrant regular articles or the priority handling given to Rapid Communications; however, the same standards of scientific quality apply. (Addenda are included in Brief Reports.) A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Energy relaxation in discrete nonlinear lattices

A. Bikaki and N. K. Voulgarakis
Department of Physics, University of Crete, P. O. Box 2208, 71003 Heraklion, Crete, Greece

S. Aubry* and G. P. Tsironis†
Center for Nonlinear Studies, MS-B258, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 17 July 1998)

We numerically investigate energy relaxation in discrete nonlinear lattices in one and two spatial dimensions. We find that energy relaxation follows a stretched exponential law, and we study its dependence on the initial temperature. We attribute this behavior to hierarchies of discrete breathers that relax with different time constants, leading to a hierarchy of relaxation time scales in the system. Using heuristic arguments, we derive a nonlinear diffusion equation for the local energy density of the oscillators that results in similar relaxation dynamics. [S1063-651X(98)14712-8]

PACS number(s): 63.20.Ry, 63.20.Pw

Recent investigations in dynamical properties of extended discrete nonlinear lattice systems have brought to the foreground a central concept, viz. that of a discrete breather [1–14]. The latter, also referred to as an intrinsic localized mode, is a space localized and principally time periodic lattice solution that under certain conditions can be shown to exist generically in nonlinear lattice systems. Breathers are now known to have very interesting dynamical properties that participate in a unique way in determining several macroscopic properties of the extended system. In the present Brief Report, we focus on one of these properties primarily related to nonequilibrium thermodynamic relaxation. This aspect of any macroscopic system is of paramount importance in processes involving thermal energy exchanges. The work reported herein expands and quantifies earlier work, where it was shown that breathers induce manifestly nonequilibrium thermal properties in the nonlinear lattice in a generic fashion [12]. Through extended numerical simulations, we show herein that energy relaxation of such nonlinear lattice systems is governed by stretched exponentials.

We consider a two-dimensional nonlinear lattice constituted typically of 44×44 lattice sites. The nonlinear oscillators located at each site interact linearly with their nearest neighbors through coupling constants k_x and k_y in the x and y directions of a square lattice, respectively. The Hamiltonian of the systems is

$$H=\sum_{\langle i,j\rangle}^{N}\left[\tfrac{1}{2}\dot{u}_{ij}^{2}+\tfrac{1}{2}k_x(u_{i+1,j}-u_{i,j})^2+\tfrac{1}{2}k_y(u_{i,j+1}-u_{i,j})^2+V(u_{ij})\right], \tag{1}$$

where the indexes i and j refer to the x and y direction, respectively, $u_{ij}\equiv u_{ij}(t)$ is the oscillator displacement at site (i,j), and $V(u_{ij})$ is the on-site nonlinear potential in the same location. For the present work we used the following three different on-site potentials ($x\equiv u_{ij}$):

$$V_1(x)=\frac{1}{2}x^2+\frac{1}{4}x^4, \tag{2}$$

$$V_2(x)=\frac{1}{2}[1-e^{-x}]^2, \tag{3}$$

$$V_3(x)=\frac{1}{2}\,\frac{x^2+ax^4}{1+x^2},\quad a=0.2. \tag{4}$$

The potentials $V_1(x)$ and $V_2(x)$ are the ''hard'' ϕ^4 and the Morse potentials respectively, while $V_3(x)$ was used extensively in the work of Ref. [13].

The investigation of the lattice energy relaxation closely follows the method of Ref. [12]. We initially use a Metropolis algorithm in order to bring the system to a given initial temperature T. Subsequently, we bring the system in contact with a zero-temperature bath created through two layers of border oscillators that are damped. Due to the presence of the

*Permanent address: Laboratoire Léon Brillouin, CEA-CNRS, CE Saclay, 91191 Gif-sur-Yvette Cedex, France.

†Permanent address: Department of Physics, University of Crete and Foundation for Research and Technology–Hellas, P. O. Box 2208, 71003 Heraklion, Crete, Greece.

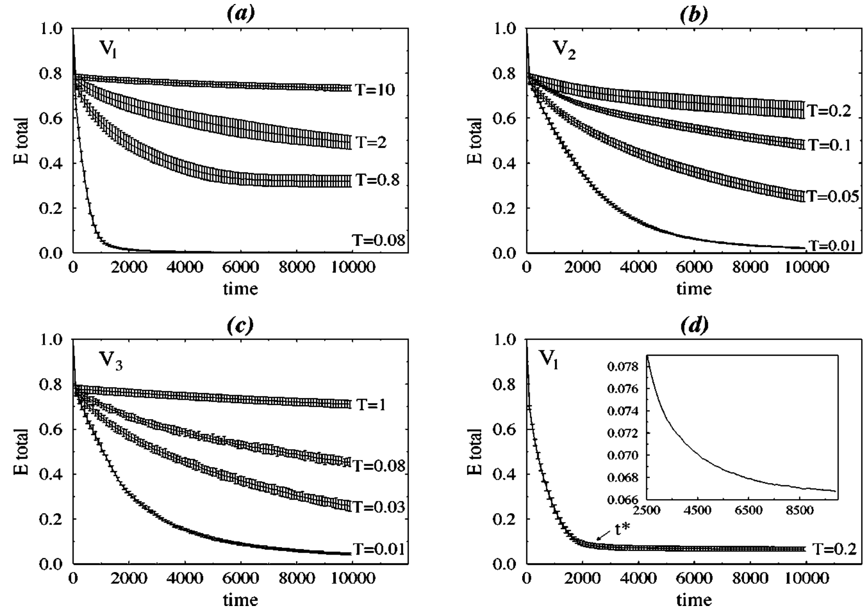

FIG. 1. Normalized energy relaxation as a function of time for potentials in (a) V_1, (b) V_2 and (c) V_3 each at four different temperatures. In (d) we plot the energy relaxation for potential V_1 with initial temperature $T=0.2$, and show the presence of a pseudocharacteristic time t^*. In the inset we show energy relaxation for $t>t^*$.

zero-temperature heat bath the nonlinear system relaxes to equilibrium (at zero temperature) following the dynamical equations of motion:

$$\ddot{u}_{ij}=k_x(u_{i+1,j}-2u_{ij}+u_{i-1,j})+k_y(u_{i,j+1}-2u_{ij}+u_{i,j-1})$$
$$-V'(u_{ij})-\gamma(\delta_{i,\mu}+\delta_{j,\mu})\dot{u}_{i,j}, \tag{5}$$

where δ denotes the Kronecker delta and $\mu=1$, 2, 43, and 44 are the border oscillators. The mass of the oscillators was set to unity. The equations of motion are solved using a fourth order Runge-Kutta method, and at each step we evaluate the total lattice energy. Several initial configurations are used for the averaged total energy relaxation as a function of time. Results of the normalized total energy relaxation for all three on site potentials at different lattice temperatures are shown in Fig. 1. We note that, as in the one-dimensional case, [12], there is astrong departure from an expected exponential relaxation at progresively higher initial temperatures. This occurs due to the increased stability of the breather modes with energy (temperature), leading to longer and longer relaxation time scales. The process of nonlinear lattice relaxation proceeds through a cascade of nested processes: at earlier times linear (phonon) mode transfer and dissipation occurs, while energy nonlinear modes (low energy breathers lying above the energy gap [14]) also dissipate. Subsequently, as time passes, higher and higher energy modes relax and dissipate. The hierarchy of relaxation processes is manifested empirically in a sequence of pseudocharacteristic times [15] $t_1^* < t_2^* < \cdots$, in between which the energy relaxation curve can be approximated by exponentials of the form $e^{\sigma t}$, with $\sigma=\sigma(T)$, i.e., with a temperature dependent time constant. An example of such behavior is depicted in Fig. 1(d) for the potential V_1 at an initial temperature $T=0.2$. We observe from Fig. 1(d) that at early times (in units of 100 periods of the linearized potentials) phonon dissipation takes place while breather relaxation occurs much later. We also show

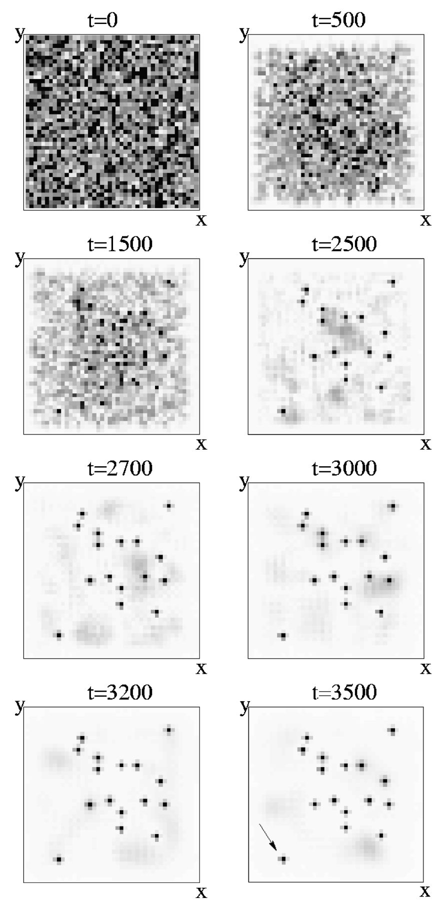

FIG. 2. Spatiotemporal breather energy landscape. We follow the approach to equilibrium of a two-dimensional lattice with on-site potential V_1 and initial temperature $T=0.2$. We plot the symmetrized local energy density (darker spots designate higher local lattice energies) in two spatial dimensions, and note the persistence of breathers to times much longer after the phonon dissipation. The arrow designates a breather whose time evolution is depicted in Fig. 3.

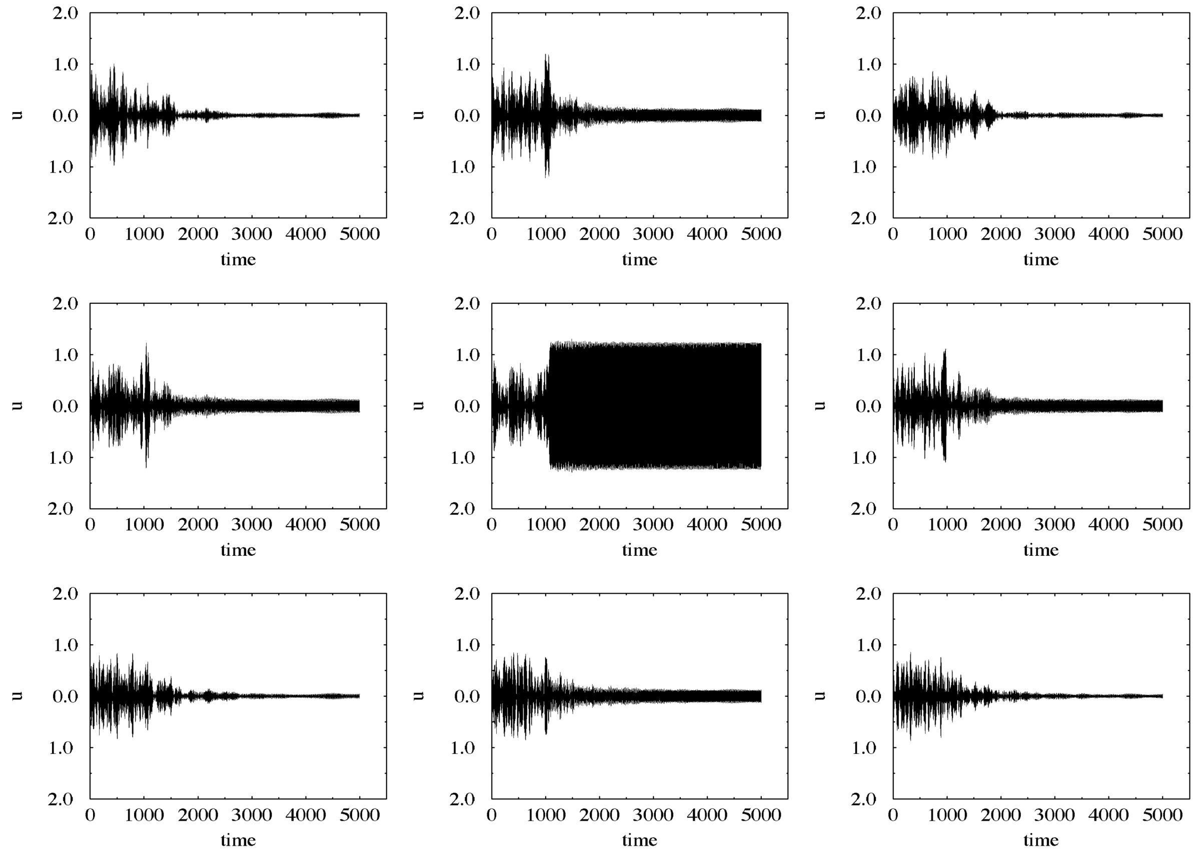

FIG. 3. Time evolution of a spontaneously generated breather event (shown with an arrow in Fig. 2) in a two-dimensional lattice with on-site potential V_1 and initial temperature $T=0.2$. We follow the central site as well as the eight sites around the dominant breather site. The coherence between the central site and the nearest neighbor sites is evident.

the slow time evolution after the pseudocharacteristic time t^* [15]. The empirical study of the lattices of the three potentials V_1, V_2 and V_3 has demonstrated that in the case of the immobile breathers of the potential V_1 a single pseudocharacteristic time t^* suffices for the characterization of the relaxation properties of the lattice (as in the case of Ref. [15]) while for the mobile breathers of the softer potentials V_2 and V_3 the relaxation process is more complex, leading to a sequence of event times.

The relative participation of linear and nonlinear modes in energy relaxation for the hard V_1 potential is seen clearly in Fig. 2, while in Fig. 3 we focus on a specific lattice neighborhood occupied by a localized breather mode and and follow its time developement. We notice the relative robustness of the breather mode once formed, and the very slow dissipation of the adjacent sites.

Extensive numerical simulations with all three potentials and use of χ^2 fitting has shown that the following stretched exponential form fits the energy relaxation curves well,

$$E(t)=E(0)e^{-\alpha t^{\beta}}, \tag{6}$$

where the coefficients α and β are temperature dependent. The best fits for $\alpha=\alpha(T)$ and $\beta=\beta(T)$ for the three potentials considered here are shown in Fig. 4 as a function of the initial temperature T. We note that the fit for the hard-ϕ^4 potential V_1 was better ($\chi_1^2\approx 10^{-5}$) than the corresponding one for V_2 ($\chi_2^2\approx 10^{-4}$). We found that both curves $\alpha(T)$ and $\beta(T)$ are well fitted by the following function:

$$f(T)=\frac{c}{1+\left[\dfrac{T}{T_0}\right]^p}+d, \tag{7}$$

where $\chi^2\approx 10^{-4}$. While the exponent p as well as the parameters c, d, and T_0 vary depending on the potential used, it is remarkable that a single functional expression fits well both the temperature-dependent exponenent $\beta(T)$ as well as the prefactor $\alpha(T)$.

An intuitive model for statistical energy relaxation in a breather infested system would have to take into account the observed fact that the energy transfer rate from a breather site to adjacent sites diminishes with the energy disparity between the sites. Considering for simplicity the one-dimensional case and denoting by ρ_n the energy density at a lattice site n, we can postulate a rate equation for the energy randomization process as

$$\dot{\rho}_n=f(\rho_{n+1}-\rho_n)(\rho_{n+1}-\rho_n)+f(\rho_{n-1}-\rho_n)(\rho_{n-1}-\rho_n), \tag{8}$$

where $f(x)$ is an appropriate even function.

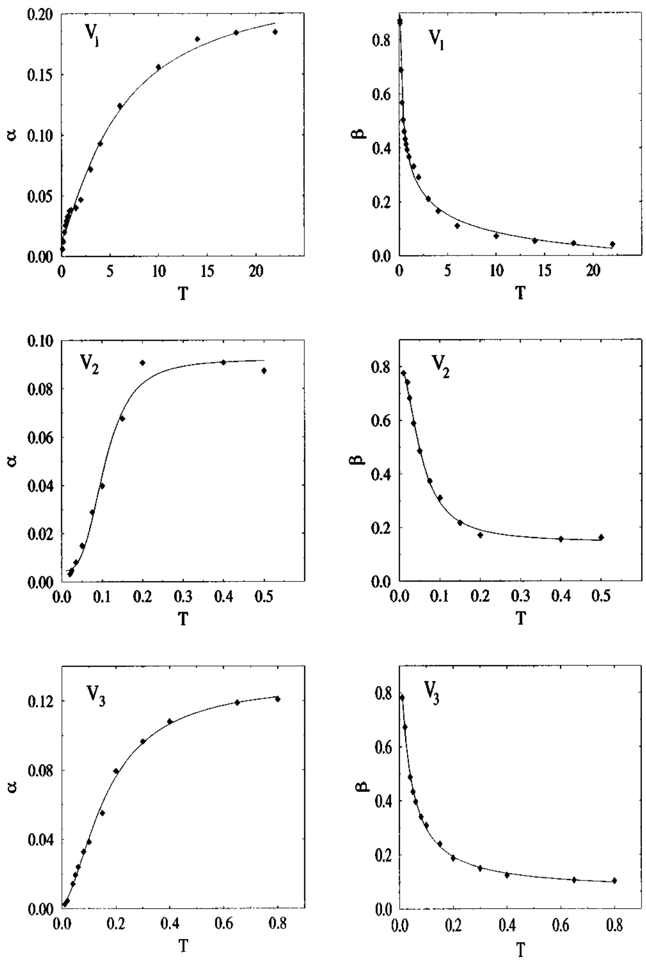

FIG. 4. Numerical data and best fits for the stretched exponential parameters α (left column) and β (right column) for all three potentials V_1, V_2, and V_3 (from top to bottom) as a function of temperature T.

Assuming as a first step a continuum limit where $\rho_n(t)$ turns into $\rho(x,t)$, Eq. (8) becomes a nonlinear diffusion equation of the form

$$\rho_t = (f(\rho_x)\rho_x)_x, \tag{9}$$

where subscripts denote differentiations with respect to the corresponding variable, and the nonlinear function $f(\rho_x)$ should be a monotonously decreasing function. It is known that nonlinear diffusion equations of this type and similar types result in algebraic time evolutions and posses self-similar solutions [16]. We thus find that the emerging picture of energy diffusion in extended nonlinear systems is one involving nonstandard relaxation [17], multiple time scales, and multifractality, as also was seen from the simulation. These properties would possibly lead to unconventional energy scaling with the system size, a feature that have been observed in lattices with long range interactions [18].

Numerical experiments with one- and two-dimensional nonlinear lattice systems have shown that the presence of breathers induces a stretched exponential lattice energy relaxation in the system. This law stems from the hierarchical relaxation processes that occur in these complex extended systems. The stretched nature of the exponential relaxation signifies that the dynamical processes involving nonlinear localized modes have fractal or multifractal natures that need to be explored. Furthermore, the heuristic connection with a porous mediumlike relaxation corroborated the complex, multifractal nature of the processes involved. The results from numerical experiments presented here call for a statistical theory that will explain the specific temperature relaxation laws of extended nonlinear lattice systems.

Partial support of INTAS 96-0158 is acknowledged.

[1] D. K. Campbell and M. Peyrard, Physica D **18**, 47 (1986).
[2] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[3] T. Dauxois and M. Peyrard, Phys. Rev. Lett. **70**, 3935 (1993).
[4] S. Aubry, Physica D **71**, 196 (1994).
[5] R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[6] K. Ø. 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 D **92**, 140 (1996).
[9] S. Aubry, Physica D **103**, 201 (1996).
[10] J. L. Marin and S. Aubry, Nonlinearity **9**, 1501 (1994).
[11] Ding Chen, S. Aubry, and G. P. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996).
[12] G. P. Tsironis and S. Aubry, Phys. Rev. Lett. **77**, 5225 (1996).
[13] D. W. Brown, L. Bernstein, and K. Lindenberg, Phys. Rev. E **54**, 3352 (1996).
[14] S. Flach, K. Kladko, and R. S. MacKay, Phys. Rev. Lett. **78**, 1207 (1997).
[15] K. Y. Tsang and K. L. Ngai, Phys. Rev. E **54**, R3067 (1996).
[16] D. G. Aronson, in *Nonlinear Diffusion Problems*, edited by A. Fasano and M. Primicerio (Springer-Verlag, Berlin, 1986).
[17] P. Allegrini, P. Grigolini, and A. Rocco, Phys. Lett. A **233**, 309 (1997).
[18] C. Anteneodo and C. Tsallis, Phys. Rev. Lett. **80**, 5313 (1998).