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Aging phenomena in nonlinear dissipative chains.

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Abstract. We study the energy relaxation in a one-dimensional nonlinear lattice with dissipative couplings. After thermalisation of this system, the extremities of the chain are put in contact with a zero-temperature reservoir, showing the existence of surprising quasi-stationary states with non zero energy, though the dissipative coupling is high. This strange behavior, due to long-lived nonlinear localized modes, induces stretched exponential relaxation laws. Furthermore, we observe a strong dependence on the waiting time t_w after the quench of the two-time intermediate correlation function $C(t_w+t, t_w)$. This function can be scaled onto a master curve, similar to the case of spin or Lennard-Jones glasses.

Keywords:

Localization of energy, Breather modes, Stretched exponential, Lattices, Aging.

PACS.

05.20.-y Classical statistical mechanics

05.45.-a Nonlinear dynamics and nonlinear dynamical systems

1 Introduction

The existence of spatially localized nonlinear excitations is old and well-known, and has been extensively studied in partial differential equations and in many experimental systems. However, this topic has been completely reactivated in the beginning of the 90's by the discovery of the striking properties of "discrete breathers". These localized and oscillating modes, solutions of discrete lattices, were discovered [1] in 1974 but the understanding of their generality in nonlinear multi-dimensional lattices is due to Takeno and Sievers [2] in 1986. Later, breathers have been shown to be spontaneously generated [3] in thermalised systems, and finally, Aubry and MacKay have proved [4] rigorously the existence of discrete breathers, exact solutions of some discrete lattices. This has initiated a period of great activity about the conditions of existence, and of stability of these modes but also about their possible applications in real systems. Experimental evidences of such excitations have thus been reported in materials [5], magnetic chains [6] and series of Josephson Junctions [7].

One of the important feature of these excitations is that they modify strongly the energy relaxation [8,9] and induces non-equilibrium dynamics. For instance in nonlinear systems where breathers are mobiles, they could contribute directly to the energy transfer and modify relaxation properties in a nonexponential dependance. This interesting phenomenon has been invoked in several physical

settings such as, DNA molecules [10], hydrocarbon structures [11], targeted energy transfer between donors and acceptors in biomolecules [12]. When the coupling is much smaller than the nonlinearity, the presence of essentially pinned long-lived breathers in nonlinear systems blocks the energy propagation [8]. The macroscopic manifestation of this phenomenon is a very slow relaxation of the total energy, reminiscent of the long lifetime of metastable states in glassy systems observed after a quench.

The case of relaxation phenomena in nonlinear lattices with bulk dissipation has received much less attention, though experimental systems belong to this class [13]. This is the reason why, in this paper, we will examine the influence in energy relaxation of a dissipative coupling by performing numerical studies of a nonlinear model. The system, described in Section 2 and pictured in Fig. 1, corresponds to particles coupled via elastic and dissipative interactions; in addition, each particle is submitted to an on-site nonlinear potential, taking into account interactions between different subsystems. For a fixed viscous parameter γ , we examine the relaxation of energy when, after thermalization, the ends of the chain are placed in contact with a zero-temperature reservoir. Results show different kinds of energy relaxation regime which depend strongly of the dissipative terms: in particular, we show that the system can relax very slowly in spite of high dissipative couplings!

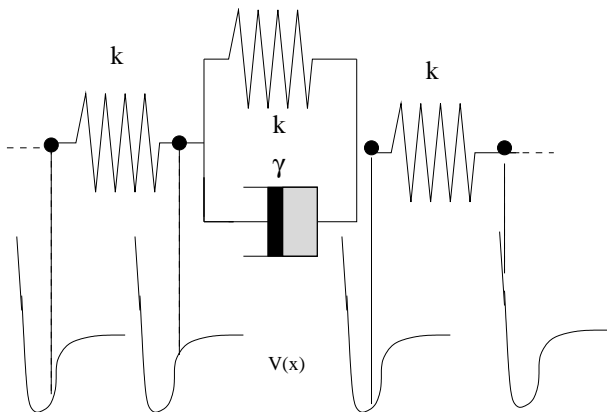


Fig. 1. Sketch of the non-linear dissipative model.

2 The dissipative nonlinear chain

We consider a one dimensional chain of $N=200$ anharmonic oscillators, with a nonlinear on-site potential $V(x)$, with free ends and nearest-neighbor elastic coupling potential (the coupling being k). The sketch of the chain is reported in Fig. 1. In order to represent the clamping degree of freedom, we consider for one half of nearest-neighbors a dissipative coupling (γ is the dissipative parameter) in parallel with elastic coupling. For the on-site potential $V(x)$, describing the interactions between two sub-units, we have chosen the Morse potential

$$V(x) = \frac{1}{2}[1 - e^{-x}]^2 \quad (1)$$

which has the appropriate shape to describe the strong repulsion when the units are pushed toward each other ($x < 0$) and the vanishing interaction when the units are pulled very far apart ($x \gg 1$). Each end oscillators of our chain can be also submitted to an additional damping force. The equations of motion of this chain are given in dimensionless form by:

$$\ddot{x}_{2i} = -\frac{\partial V}{\partial x_{2i}} - k(2x_{2i} - x_{2i+1} - x_{2i-1}) - \gamma(\dot{x}_{2i} - \dot{x}_{2i-1}) - \gamma'\dot{x}_{2i} \delta_{2i,200} \quad (2)$$

and

$$\ddot{x}_{2i+1} = -\frac{\partial V}{\partial x_{2i+1}} - k(2x_{2i+1} - x_{2i} - x_{2i+2}) - \gamma(\dot{x}_{2i+1} - \dot{x}_{2i+2}) - \gamma'\dot{x}_{2i+1} \delta_{i,0} \quad (3)$$

where x_n is the dimensionless displacement of the n th oscillator from equilibrium, \dot{x}_n its velocity and δ the Kronecker delta function. The mass of the oscillators is set to unity by appropriately renormalizing time units. γ' corresponds to the damping coefficient of a surrounding heat bath, described below.

To study energy relaxation, we consider $k=0.01$ and we initially thermalize the system at temperature $T=1$ by using Nosé-Hoover thermostats [14]. This temperature is much higher than the critical temperature ($T_c=0.2$) of the

"order-disorder" transition which characterizes the non dissipative model $\gamma=0$ (for more detail see references [15, 16]). Then, in average, the kinetic energy per site is higher than the depth of the Morse potential (which is equal to 0.5 in our arbitrary units): we can therefore consider our system as in an initial "liquid" state: all the particles are in the plateau of the Morse potential. In other words, there are no interaction between units. The thermalization procedure is performed with $\gamma=\gamma'=0$ by using a chain of three thermostats to provide a good exploration of the phase space [14]. The equations of motion have been integrated using a fourth order Runge-Kutta method with timestep 0.01.

After thermalization, the connection with the heat bath is turned off and the lattice is connected to a zero temperature reservoir via the damping term with $\gamma'=0.1$. Instead, the dissipative parameter γ varied in the interval $[0,100]$. The moment of connection with the zero temperature reservoir is chosen as the origin of time. At each step of the integration of equations (2) and (3), we evaluate the total lattice energy:

$$E = \sum_{i=1}^{200} \left[\frac{1}{2} \dot{x}_i^2 + V(x_i) \right] + \sum_{i=1}^{199} \frac{k}{2} (x_{i+1} - x_i)^2 \quad (4)$$

and consider the symmetrized local energy per site:

$$E_i = \frac{1}{2} \dot{x}_i^2 + V(x_i) + \frac{k}{4} (x_{i-1} - x_i)^2 + \frac{k}{4} (x_i - x_{i+1})^2 \quad (5)$$

Total energy is expected to decrease with time and converge to a zero value of the "frozen" state at equilibrium.

3 Relaxation of the thermalized system

In Fig. 2, we report the total lattice energy divided by the initial energy versus time for various viscous parameter γ . For $\gamma=0$, a clear non exponential decreasing energy is observed, consistent with Tsironis and Aubry's results [8]. This long-tail relaxation behavior was shown by these authors to be connected to the presence of long-lived non linear localized modes that are relatively mobile. If we consider a small dissipative coupling ($\gamma=10^{-3}$) inside the lattice, we see that total energy decreases faster than previously. This small dissipative coupling induces a strong modification of energy relaxation to the "frozen" state (normalized energy closed to 0) for a time smaller than 10^4 (in arbitrary units). This emphasizes that the dissipative couplings change strongly the relaxation mechanisms and can induce a fast relaxation regime.

For γ higher than 0.1, a new surprising feature is observed: normalized energy seems to be blocked with a very slow decrease for long time whereas the dissipative parameter is higher! The system seems to evolve in a quasi-stationary state that is neither a "frozen" state (the normalized energy is clearly different from 0) nor a "liquid" state" (energy is too low). We can also notice that, at a given time, the energy of this quasi-stationary state

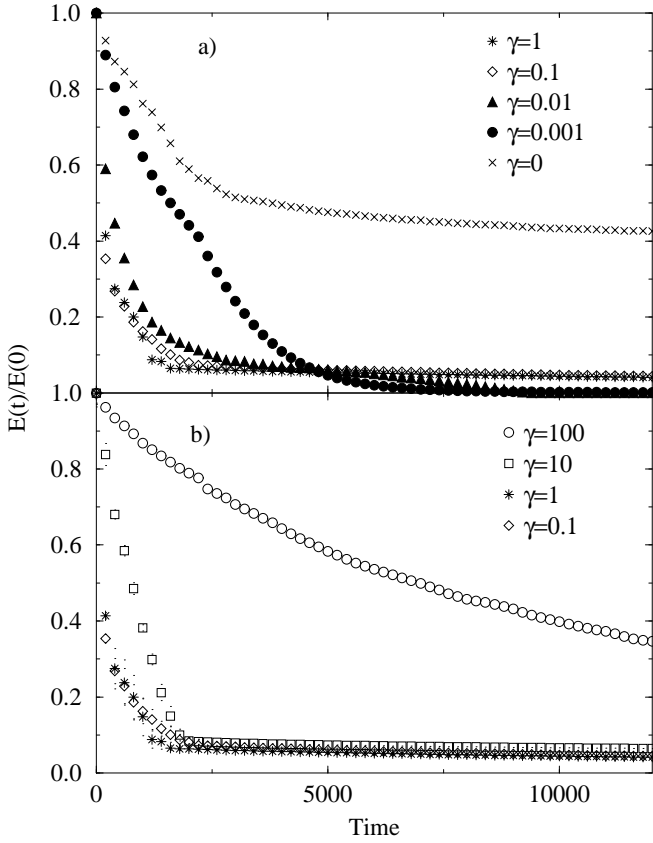


Fig. 2. Normalized total energy decay as function of time for various viscous parameter γ . Initially each array is in thermal equilibrium at the temperature $T=1$.

increases with γ . This situation is reminiscent of polymer systems where very long-lived non-equilibrium aging states are observed.

In previous relaxation studies in non linear lattices where blocking energy was observed, it has been shown that such behavior may be induced by long-lived breathers [8]. In order to examine more precisely the present situation, we report in Fig. 3 the spatiotemporal energy landscape of the lattice by plotting the local energy E_i in each lattice site for $\gamma = 10^{-3}, 10^{-1}$ and 10. Time advances along the y axis until $t=10^4$ and a gray scale is used to represent the local energy with darker shading corresponding to more energetic regions. In the case $\gamma=10^{-3}$, Fig. 3c emphasizes two kinds of energy relaxation: on the one hand, there is a dissipation of energy inside the lattice, characterized by a "fibrous structure" of the local energy landscape; on the other hand, we observe a dissipation of mobile breathers via surface damping characterized by "dark oblique lines". For $\gamma \geq 0.1$, we notice the clear presence of pinned long-lived breathers, responsible of the energy relaxation blocking. This localisation of energy is observed after a short time where energy not only decreases via the surface damping but also via a dissipation inside the lattice (see for example the landscape for $\gamma = 10^{-1}$ and $t < 2500$). Furthermore, these states have a very long lived time and are still observed for t higher than 10^5 .

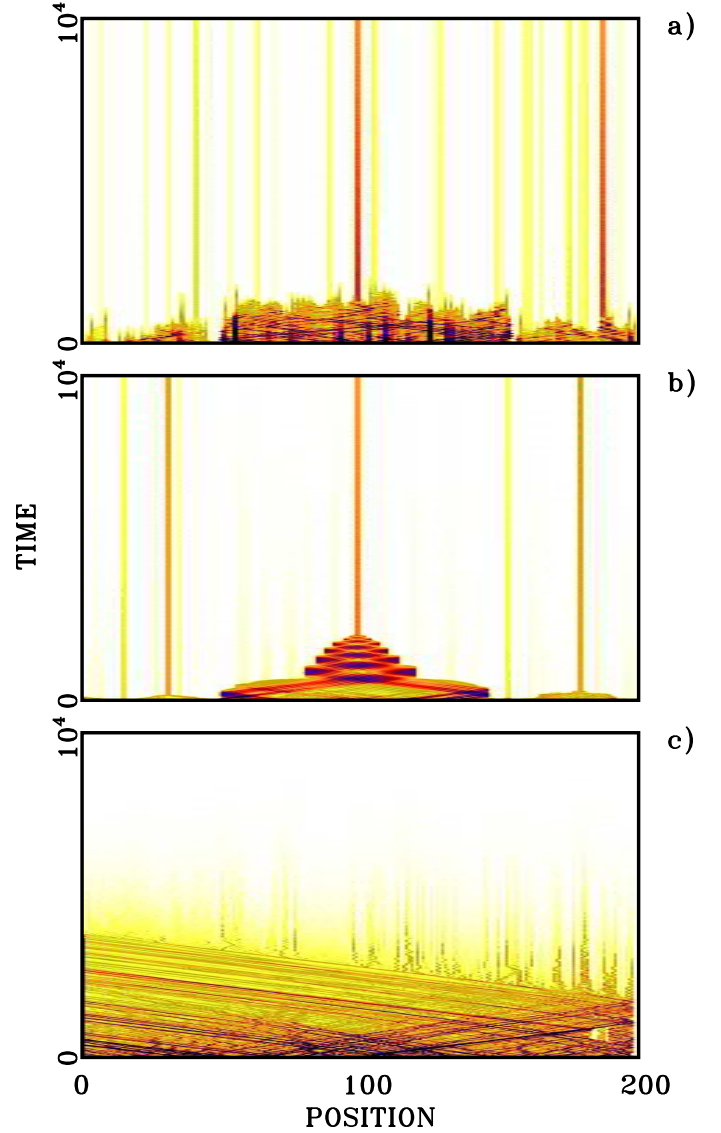


Fig. 3. Evolution of the local energy E_i along the chain for various viscous parameter $\gamma=10$ (panel a), 0.1 (panel b) and 0.001 (panel c). The grey scale goes from $E_i=0$ (white) to the maximum E_i -value (black).

We have mentioned previously that, at early times, phonon and mobile breather dissipation takes place before pinned breathers relaxation. Typically the hierarchy of relaxations processes may be classified in a sequence of characteristic times $t_1^* < t_2^* < \dots$ [17], where the energy relaxation corresponds approximately to exponential or stretched exponential decay [18]. Let us introduce the phonon relaxation time t^* defined by $E(t^*)/E(0)=0.5$ which is characteristic of the phonon and mobile breather dissipation inside the lattice. We have reported in Fig. 4 the evolution of this relaxation time versus the viscous parameter γ . We clearly see, in this first step, that energy decreases faster for γ between 0.1 and 1. In the case of a linear lattice, the maximum of dissipation is predicted to correspond to a value of γ which verifies $\gamma\omega \sim K + k$ where K corresponds to the coupling constant of the linearized Morse potential

($K=1$ in our case) and ω is the frequency of the phonon band that starts at the frequency $\sqrt{K}=1$ and extends to $\sqrt{K+4k}\sim 1.02$. Therefore, in the case of linearized oscillator, we expect a maximum of dissipation for γ close to 1 in agreement with what is reported in Fig. 4. It is thus surprising to observe quasi-stationary states in a second regime whereas dissipative effects are important, even the presence of slow relaxation when the friction is large is reminiscent of the behavior of damped harmonic oscillators.

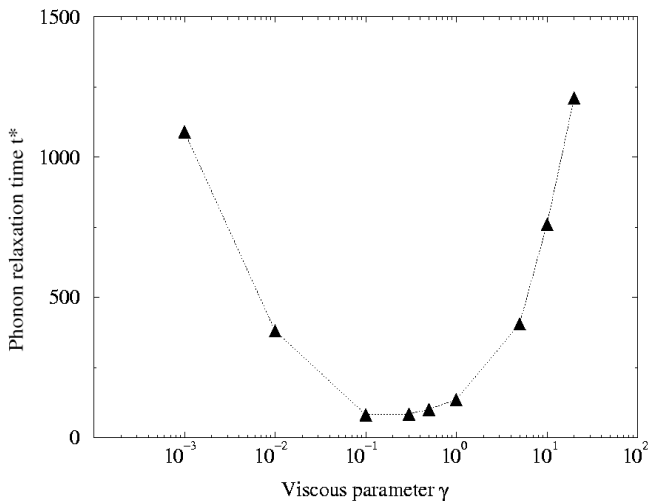


Fig. 4. Phonon relaxation time t^* , defined by $E(t^*)/E(0)=0.5$, for various values of the viscous parameter γ .

In Fig. 5, we report the local energy in the lattice for various parameter γ and at a given time $t=2\cdot 10^4$ much higher than the characteristic time of phonons and mobile breathers dissipation. For $\gamma < 0.1$, the local energy per site is close to 0 as seen previously in Fig. 2: the system with small dissipative coupling reached thus rapidly an equilibrium frozen state. For $\gamma \geq 0.1$, we clearly see the localization of energy, as long-lived breathers, corresponding to two nearest-neighbors oscillators, vibrating in phase, but distributed evenly on the lattice. We have verified that the two considered nearest-neighbors are coupled via piston: when γ is high enough this coupling is clamped. In fact, the phase displacement of velocities of both particles is very small, inducing a very slow dissipation and therefore a very long-lived out-of-equilibrium state. The energy of these long-lived breathers is close to 0.5 at time $t=2\cdot 10^4$, and the associated sites are not linked with the on-site Morse potential. This quasi-stationary state is clearly not a frozen state, since some parts of a molecular chain are "hot" but do not interact with other ones.

For $t \gg t^*$ and $\gamma \geq 0.1$, the energy relaxation of the quasi-stationary state can be very well fitted by a Kohlrausch-Williams-Watts function or stretched exponential function:

$$E(t) = E_b(0)e^{-(at)^b} \quad (6)$$

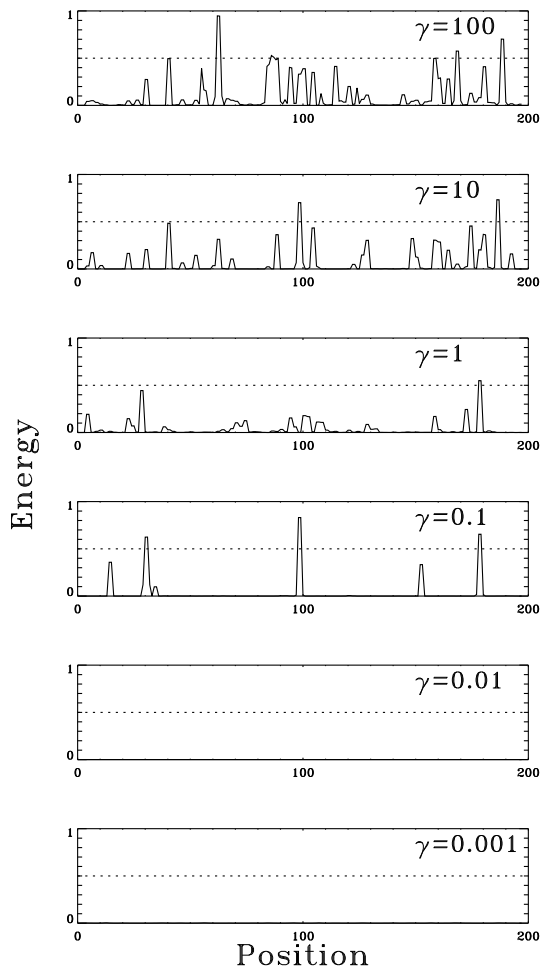


Fig. 5. Instantaneous local energy E_i along the chain at time $t=2\cdot 10^4$ for various dissipative parameter γ . The dashed lines show the limit of Morse potential for large displacement x_i .

where the coefficients a , b and $E_b(0)$ are γ dependent. $E_b(0)$ can be qualified as the total energy of pinned breathers at time $t=0$. The Kohlrausch [19] exponent b is a parameter measuring the deviation from a single exponential form ($0 \leq b \leq 1$). In Fig. 6, we have reported the evolution of $-\ln[E(t)/E_b(0)]$ versus t with logarithmic scales for various parameter $\gamma \geq 0.1$. We see a very clear linear dependence for high t (after phonon and mobile breather dissipation), which attests that this long-lived breather energy relaxes as a stretched exponential.

We see also in these figures that the slope of the straight lines depends on the viscous parameter γ . In order to examine more precisely this dependence, we report in Fig. 7 the Kohlrausch exponent b versus the viscous parameter γ . The error bars are shown in the picture, but are hidden by the symbols, suggesting that the fit is very good. We clearly see a maximum of the exponent b for values of γ close to 0.5. The b -value is equal to 0.82 and then the energy relaxation differs from a pure exponential decay. Furthermore, this figure shows that the pinned breathers relaxation is slower for higher parameter γ .

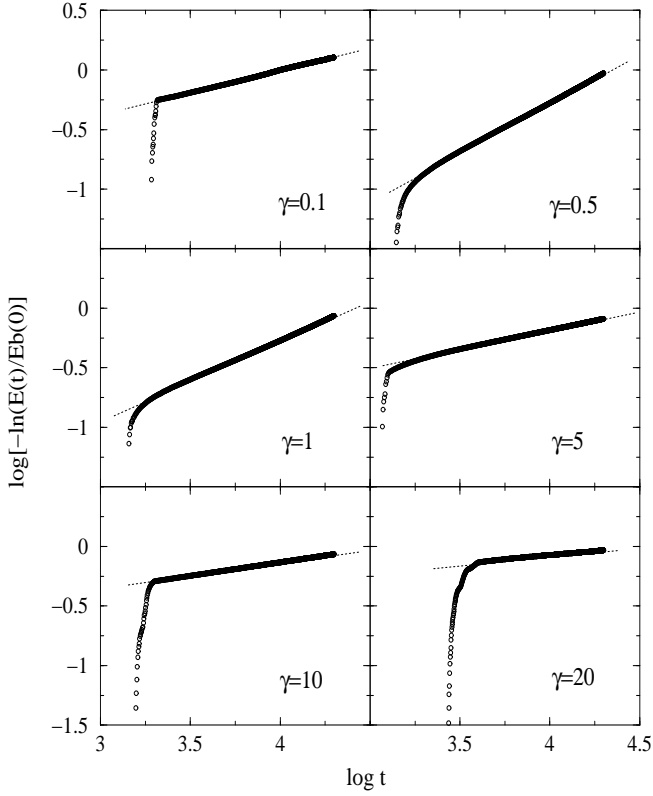


Fig. 6. $\log[-\ln(E(t)/E_b(t))]$ versus $\log t$ for various dissipative parameter γ . The dotted lines are the stretched exponential fits.

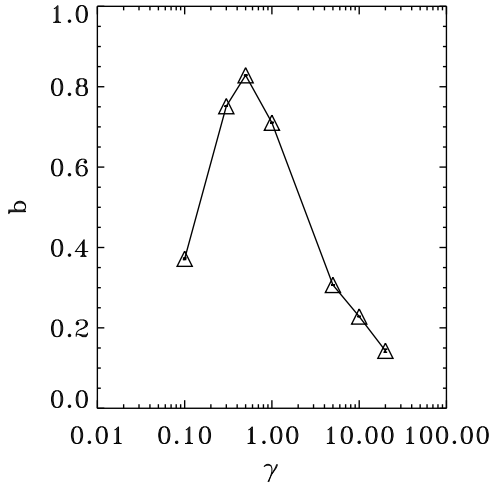


Fig. 7. Kohlrausch exponent b for various viscous parameter γ .

4 Out of equilibrium dynamic correlations

Studies of nonequilibrium systems like spin, structural or Lennard-Jones glasses [20, 21] have shown that the nonequilibrium dynamics of the previously described states could be much efficiently characterized by two-time correlation

functions of the form [26]:

$$C(t_w + t, t_w) = \langle A(t_w + t)A(t_w) \rangle - \langle A(t_w + t) \rangle \langle A(t_w) \rangle \quad (7)$$

where A is a microscopic observable, and t_w is the "waiting time" i.e., the time elapsed after the quench. Brackets denote an average over different initial configurations at temperature T . At equilibrium, this two-time quantity satisfies time translation invariance and then depends only on the time t . On the other hand, in out of equilibrium situations, such equilibrium property is not verified: this function depends on the waiting time t_w ("aging effect"). The correlations functions for large times are expected to scale in the form:

$$C(t_w + t, t_w) = C_{ST}(t) + C_{AG} \left(\frac{\xi(t_w + t)}{\xi(t_w)} \right). \quad (8)$$

The first term describes short time dynamics that does not depend on t_w and has the equilibrium form. The second term, or aging part, depends only on the ratio $\xi(t_w + t)/\xi(t_w)$ where $\xi(t)$ is a monotonous increasing function of t . In a lot of cases $\xi(t) \propto t$ or $\propto t^\nu$ so that the aging part is simply a function of t/t_w and exhibits a master curve (see for instance, experiments on thermoremanent magnetization [22], gels [23] or particle suspensions [24, 25]).

In this study we have considered the microscopic observable $A(t) = (\sum_{i=1}^{200} x_i(t))/200$ that is the mean deformation per site of the chain at time t . Numerical calculations have been done in the case of a quench of the system with a viscous parameter $\gamma=10$ from temperature $T=1$ to $T=0$. Two-time correlation functions are obtained for various waiting time by considering 11 different initial configurations. Furthermore, in order to make a quantitative comparison, we prefer to calculate correlation normalized by $C(t_w, t_w)$.

In Fig. 8, we have reported the evolution of normalized two-time correlations function $C(t_w + t, t_w)$ versus time t for different waiting time (we consider $t_w \gg t^*$ in order to study only long lived non equilibrium states after phonons and mobile breathers dissipation). The behavior of C clearly emphasizes the lost of time-translation invariance and the dependence on the waiting time t_w . This figure also shows that the dynamics can be decomposed into two time scales:

(i) at short time separation ($t < 20$) correlation function doesn't depend on t_w and is equal to the value expected at equilibrium ($C=1$ at $T=0$).

(ii) the decay from this value toward zero arises in a second time scale that clearly depends on t_w : the system doesn't reach equilibrium within the time window explored in the simulation. Furthermore we can notice that the larger the waiting time, the longer it takes the system to forget the configuration at time t_w . This behavior is typical of aging effect [20].

Guided by equation (8) we test the scaling assumption for long times in Fig. 9, where normalized correlation functions are reported versus normalized time t/t_w . The different curves can be superimposed, indicating the validity

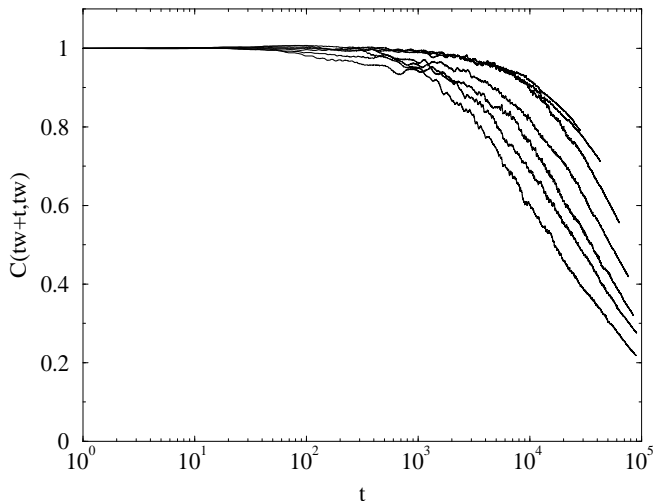


Fig. 8. Normalized non-equilibrium correlation function $C(t_w+t, t_w)$ for fixed value t_w versus time t . The viscous parameter is $\gamma=10$ and from bottom to top the waiting times are $t_w=5844, 9300, 14700, 23137, 36321, 56920, 71225$.

of the scaling ansatz and the existence of a master curve. This striking feature is observed in many non-equilibrium systems [22–25] and is very similar with comparable studies on spin glasses [20] or Lennard-Jones glasses [21]. The physical origin of this universal t/t_w scaling is, at this day, an open question. Kob and Barrat suggest in reference [21] that it could be induced by a similarity of the geometry of phase space of these systems in spite of differences in microscopic dynamics.

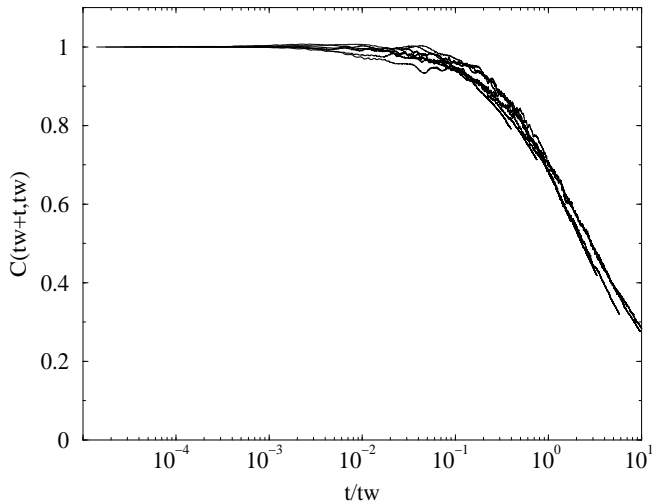


Fig. 9. The data of Fig 8 versus t/t_w : master curve

Finally, we would like to point out that Fig. 8 shows also the violation of the dissipation-fluctuation theorem (FDT). It seems to be a characteristic of non-equilibrium system as observed numerically in domain growth process [27], Lennard-Jones glasses [28] or slow granular rheology [29] and experimentally for dielectric measurements

in colloidal glasses [30], supercooled fluid [31] and polymer glasses [32,33]. Let us consider the response $R(t_w+t, t_w)$ to a field h conjugated to observable A . For systems out-of-equilibrium, response to an external field is given by the following equation:

$$\begin{aligned} R(t_w+t, t_w) &\equiv \left. \frac{\delta \langle A(t_w+t) \rangle}{\delta h(t_w)} \right|_{h=0} \\ &= -\frac{\chi(C)}{T} \frac{\partial C(t_w+t, t_w)}{\partial t} \end{aligned} \quad (9)$$

where $\chi(C)$ is a phenomenological function. We thus obtain:

$$\frac{\partial C(t_w+t, t_w)}{\partial t} = -\frac{T}{\chi} R(t_w+t, t_w) \quad (10)$$

where T is the bath temperature. Obviously, for equilibrated systems, $\chi(C)$ is equal to 1 and the FDT is recovered.

If we consider a quench with a *zero-temperature bath*, then for satisfying FDT, the derivative of the normalized correlation function has to vanish. Just after the quench, as usual, this requirement would not be fulfilled during the time for equilibration which is clearly independent of the waiting time. However, in the present nonlinear dissipative model, evolutions of correlation functions reported in Fig. 8 show clearly that convergence toward the regime where the FDT is correct, depends on the waiting time t_w . Consequently FDT is violated in this non-equilibrium system as seen in other glasses [27–33]. Moreover, the larger the waiting time, the longer the FDT is violated by the system.

5 Conclusion

We have studied a one dimensional nonlinear lattice characterized by dissipative couplings. The energy relaxation studies of this thermalized system show that for sufficiently large viscous parameter γ , it is possible to observe nonequilibrium quasi-stationary states in spite of the short characteristic time of phonon dissipation! This surprising behavior is due to a chain auto-organisation which minimizes energy dissipation, inducing the clamping of some degrees of freedom and forming long-lived pinned breathers.

Moreover, this very slow energy relaxation can be fitted by stretched exponential laws, ubiquitous in glassy polymer aging properties. Another similarity with these physical systems is that this aging phenomenon is slower when the viscous parameter γ is higher. Furthermore, the two-time correlation function $C(t_w+t, t_w)$ shows a strong dependence on the waiting time and can be scaled onto a master curve by considering the evolution versus normalized time t/t_w .

By these aspects (clamping of degree of freedom, long-lived nonequilibrium state, stretched exponential decays, violation of time-translation invariance and master curve), the aging nature of this simple dissipative non linear lattice is very similar to those observed in glassy polymers.

Beside its interest for nonlinear physics, this model is presumably an alternative to study complex systems like glassy state polymers: we have now to push our investigations further by examining other properties like dependences on cycling temperature, evolution with waiting time of the elastic moduli.

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