THERMAL ACTIVATION OF BREATHERS IN 2D NON–LINEAR LATTICES

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We study the energy relaxation process produced by damping 2D lattices of classical anharmonic oscillators at the edges. Spontaneous emergence of localised vibrations dramatically slows down dissipation and gives rise to quasi–stationary residual states where energy is trapped in the form of a gas of weakly interacting discrete breathers. We show that the existence of a gap in the breather spectrum in 2D causes the localisation process to become activated. We investigate such a mechanism by studying the localisation time and the average density of localised objects.

Nonlinearity has revealed one of the key ingredients for describing many relevant features of different states of matter. Recently, considerable efforts have been devoted to the study of periodic, localised, non–linear lattice excitations named "breathers" [1], which emerge in non–linear systems from the interplay of non–linearity and space discreteness [2]. The role of discrete breathers in non–equilibrium dynamics seems to be particularly fascinating. An example is the relaxation to energy equipartition of short–wavelength fluctuations [3]. Another interesting scenario where breathers are found to emerge spontaneously is observed upon cooling a thermalised lattice at its boundaries [4,5,6,7] .

The mechanisms leading to spontaneous localisation are intimately related to how dissipation acts on linear modes of different wavelengths [6]. In particular, modulation instability of short lattice waves [8] is the mechanism underlying the birth of breathers from an interacting gas of solitons [3,9]. In

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2D the result is a multi–breather quasi–stationary state, where breathers are static and close–packed in a "random" lattice, and whose decay is exponential with a huge time constant (of the order of the breather's amplitude at the lattice edges) [7]. In addition, the existence of an energy activation threshold for breather solutions [10] leads to conjecture that a thermalised lattice may be cooled down to the residual state only above some initial energy, making spontaneous localisation of energy in 2D a fluctuations–activated process.

In this contribution, we concentrate on the characteristics of the relaxation dynamics that confirm the thermal activation hypothesis. We consider a $N \times N$ lattice with one degree of freedom per site and damping on all edges. The atoms are labelled by the indexes $i, j = 0, 1, \dots, N-1$ and we denote with $u_{i,j}$ the displacement of the particle at site (i, j) from its equilibrium position. The lattice dynamics is given by the following equations of motion

$$\begin{aligned} \ddot{u}_{i,j} = {} & V'(u_{i+1,j} - u_{i,j}) - V'(u_{i,j} - u_{i-1,j}) + \\ & V'(u_{i,j+1} - u_{i,j}) - V'(u_{i,j} - u_{i,j-1}) - \sum_{p,q=0}^{N-1} \Gamma_{i,j}^{p,q} \dot{u}_{p,q} \quad . \end{aligned} \tag{1}$$

Here $V(x) = x^2/2 + x^4/4$ is the Fermi-Pasta-Ulam (FPU) potential and $\Gamma_{i,j}^{p,q} = \gamma[g_{i,p}\delta_{j,q} + \delta_{i,p}g_{j,q} - g_{i,p}g_{j,q}]$, with $g_{i,p} = \delta_{i,p}[\delta_{p,0} + \delta_{p,N-1}]$, is the damping matrix, γ being the damping rate. We take here free–ends boundary conditions (BC), since localisation is strongly inhibited by fixed–ends BC [6].

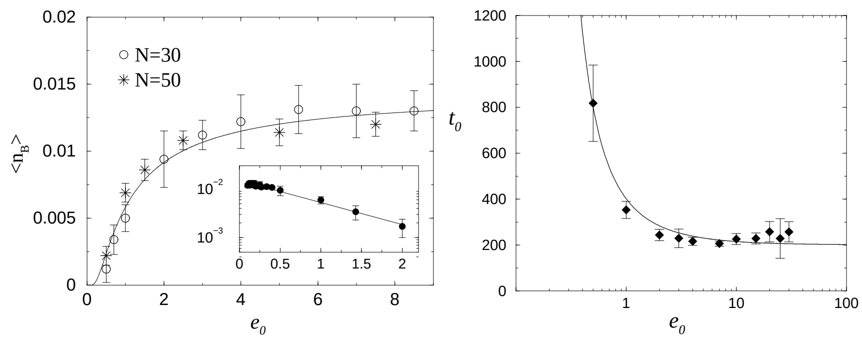
It is possible to confirm the thermal activation hypothesis by performing a statistical analysis of the residual state. In particular, we find that the average density of localised objects follows an Arrhenius law of the form [7]

$$\langle n_B \rangle \propto \exp(-\beta\Delta) \quad , \tag{2}$$

where $1/\beta$ is proportional to the initial energy density $e_0 = E(0)/N^2$ (Fig. 1 (a))

A further confirmation of the thermal activation hypothesis comes from a phenomenological analysis of the localisation pathway. The transient regime leading to the residual state can be studied by looking at the localisation parameter L, defined as

$$L(t) = N^2 \sum_{i,j} h_{i,j}^2(t) \Bigg/ \left[\sum_{i,j} h_{i,j}(t) \right]^2 \quad , \tag{3}$$



(a) (b)

Figure 1. 2D FPU lattice, $\gamma = 0.1$. (a) Average breather density $\langle n_B \rangle$ vs initial energy density for $N = 30$ and $N = 50$ and Arrhenius plot. The inset shows the average density measured in the $N = 50$ system vs $1/e_0$ in lin–log scale, and an exponential fit. (b) Localisation time t_0 vs initial energy density (symbols) and fit with Eq. (5)

where $h_{i,j}$ are the symmetrised site energies. When the lattice energy is highly localised L is of order N^2, while L order 1 means that the energy is evenly spread over the whole lattice.

We can introduce a localisation time t_0 by fitting the localisation parameter curve with the empirical function

$$L(t) = [L_0 + L_\infty (t/t_0)^\sigma]/[1 + (t/t_0)^\sigma] \quad , \tag{4}$$

where σ is a suitable exponent and $L_0 \approx 1$ and $L_\infty \approx N^2$ are the equilibrium and asymptotic values of $L(t)$, respectively (Fig. 2). From an energy–dependent analysis of the localisation curves we find that $t_0 \propto L_\infty$. On the other hand, it is not difficult to realise that in the residual state one must have

$$L_\infty \;\propto\; \langle \epsilon_B \rangle^2 \langle n_B \rangle / (\langle \epsilon_B \rangle \langle n_B \rangle)^2 \;\propto\; 1/\langle n_B \rangle \;\propto\; \exp(\beta \Delta) \quad , \tag{5}$$

where we have introduced the average breather energy $\langle \epsilon_B \rangle$. We show in Fig. 2 (b) a fit with Eq. (5) to the experimental values of the localisation time for an FPU lattice with $N = 50$.

Conclusions

We study the phenomenon of spontaneous energy localisation upon cooling in 2D lattices. We perform a statistical analysis of the pseudo–stationary

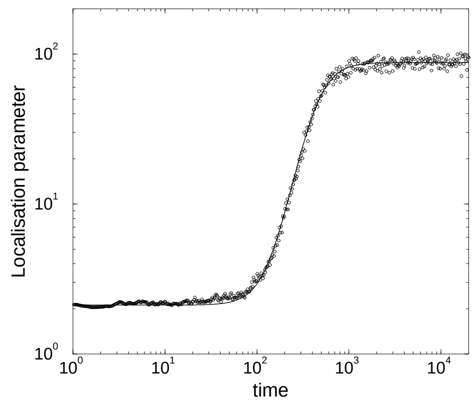


Figure 2. 2D FPU lattice with $N = 50$, $e_0 = 1$ and $\gamma = 0.1$. Localisation parameter vs time (circles) and fit with Eq. (4).

state, where spontaneously emerged breathers arrange on a static random lattice. We determine the average breather density as a function of the initial energy of the lattice and show that it is well described by an Arrhenius law. This conclusion confirms that spontaneous localisation of energy in 2D is a thermally–activated process, in accordance with the presence of an energy threshold for breather solutions in 2D. This conclusion is also confirmed by an analysis of the localisation time.

Acknowledgments

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