Stochastic metastability by spontaneous localization

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Nonequilibrium, quasi-stationary states of a one-dimensional “hard” $\phi^4$ deterministic lattice, initially thermalized to a particular temperature, are investigated when brought into contact with a stochastic thermal bath at lower temperature. For lattice initial temperatures sufficiently higher than those of the bath, energy localization through the formation of nonlinear excitations of the breather type during the cooling process occurs. These breathers keep the nonlinear lattice away from thermal equilibrium for relatively long times. In the course of time some breathers are destroyed by fluctuations, allowing thus the lattice to reach another nonequilibrium state of lower energy. The number of breathers thus reduces in time; the last remaining breather, however, exhibits amazingly long life-time demonstrated by extensive numerical simulations using a quasi-symplectic integration algorithm. For the single-breather states we have calculated the lattice velocity distribution unveiling non-gaussian features describable in a closed functional form. Moreover, the influence of the coupling constant on the life-time of a single breather has been explored. The latter exhibits power-law behaviour as the coupling constant approaches the anticontinuous limit.

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\textbf{Introduction.} - The energy relaxation of thermalized deterministic systems in close contact with temperature baths have been long investigated, and several important results have been obtained \textsuperscript{1-3}. One of the most important aspects of this problem for nonlinear systems is the non-exponential relaxation behaviour of the energy as a function of time, that has been connected to the formation of spontaneously generated discrete breathers, i.e., spatially localized and time-periodic excitations that appear generically in extended nonlinear lattices \textsuperscript{4,5,6}. The question then arises about the life-times of these entities, which result from cooling of an initially ”hot” deterministic system in contact with a thermal bath. In the present work we investigate the relaxation of energy in a deterministic nonlinear lattice comprised of $N$ nearest-neighbour coupled oscillators, that is in contact with a stochastic thermal (Langevin) bath. We demonstrate that for large initial temperature differences between this lattice and the bath, the former may not reach thermal equilibrium (eq) with subsequent equipartition of energy between its degrees of freedom but, instead, it may end up in a very long-lived metastable state with a relatively small number of breathers concentrating most of the energy. In these non-equilibrium, metastable states, we analyze the total velocity distribution of the lattice and compare it with the Gaussian one being present at thermal equilibrium. We further show that the life-time $\Delta t$ of a breather presents a power-law dependence on the strength of the coupling constant $k$ between neighboring oscillators. The slope of the former dependence is influenced by the temperature of the bath.

\textbf{Stochastic equations of motion.} - Consider a free-end, one-dimensional nonlinear lattice of oscillators (of mass $m$ equal to unity) without dissipation and external forcing, whose symmetrized Hamiltonian function is given by

\begin{equation}
H = \sum_{n=1}^{N} \left( \frac{1}{2} p_n^2 + V(x_n) \right) + k \left( \frac{1}{4} (x_{n-1} - x_n)^2 + (x_n - x_{n+1})^2 \right),
\end{equation}

where $p_n = \dot{x}_n$ is the canonical conjugate momentum of the $n$th oscillator (the overdot denotes derivation with respect to the temporal variable), $k$ is the coupling coefficient between nearest neighbouring oscillators, $N$ is the number of oscillators and $V(x_n) = \frac{a}{2} x_n^2 + \frac{b}{4} x_n^4$ is the nonlinear on-site potential, with $a$ and $b$ being positive coefficients. The values of $a$ and $b$ are set to unity throughout the paper. The resulting Hamilton’s equations of motion

\begin{equation}
\ddot{x}_n = k (x_{n-1} - 2x_n + x_{n+1}) + ax_n + bx_n^3,
\end{equation}

describe the dynamics of the displacements of that deterministic system, hereafter referred to simply as "the system". The system is initially thermalized to attain a particular temperature $T_0$ using the standard Metropolis algorithm. When the thermalization procedure is over, the system is embedded into a stochastic thermal bath (or simply "the bath") of lower temperature, say $T_b$, by adding $N_b$ stochastic oscillators at each edge of the system. The dynamics of the bath is then described by Langevin equations resulting from Eqs. \textsuperscript{2} with the addition of a stochastic and a dissipative term on the right-
hand-side, in the form

\[-γ\dot{x}_n + \sqrt{2γ}T_b ξ_n(t),\]  

where \(γ\) is the dissipation coefficient and \(ξ_n(t)\) are zero mean uncorrelated random Gaussian deviates of standard deviation unity. As usual, the Boltzmann’s constant \(k_a\) has been set to unity. The equations for the system and the bath are integrated for long times with a quasi-symplectic stochastic integrator of second order \([14–16]\).

While for the corresponding linear system the thermal equilibrium is reached exponentially fast, the presence of nonlinearity complexifies considerably the energy relaxation behaviour. Throughout this work, the temperature of the bath is calculated according to the equipartition theorem of the thermodynamic canonical ensemble, from the total average kinetic energy \(\langle E_k\rangle_{eq} = \frac{1}{2}\sum_n p_n^2\) through the relation \(\langle E_k\rangle_{eq} = \frac{1}{2}N k_a T\).

**Metastability.** - In the presence of nonlinearity, two different regimes are observed; the energy of the system either relaxes to that corresponding to the thermal equilibrium temperature \(T_b\), or it decreases slowly towards thermal equilibrium following a sequence of long-lived, metastable states (with energies higher than these at thermal equilibrium). The latter states, which are reached when the system initially has a temperature much higher than that of the bath, are due to the formation of nonlinear excitations of the form of discrete breathers. The system has initially a high amount of energy; as it cools down, a number of breathers can be formed trapping significant amounts of energy at particular, random lattice sites. These breathers become unstable and disappear in the course of time, leading to the decrease of energy in time that exhibits a staircase pattern. The aforementioned energy decay behaviour is recorded in Fig. (a) for three trajectorays, each of them corresponding to a different set of initial conditions (i.e., three different thermalizations), while all the other parameters are kept fixed. Indeed then, depending on the initial conditions the system may be either led directly to the thermal equilibrium state (black curve), or it may stay at one of the metastable states (indicated by the formation of horizontal segments characterized by constant energy, i.e., red and orange curves) until it gradually reaches \(T_b\). In Fig. (b) we plot the energy density on the site-number \(n\)-time \(t\) plane for the “orange” trajectory shown in (a).

As well known, at thermal equilibrium the velocity \(v_n\) presents a Gaussian distribution. It is interesting then to explore to which extent the former distribution changes at the various local equilibrium, metastable states. Particularly, we study the last metastable state before equilibrium corresponding to the existence of a single breather; the former state can be quickly reached by adding more edge-oscillators in the thermal bath. Therefore we choose \(N_b = 22\). Then, considering a set of initial conditions leading to equilibrium of the total energy \(\langle E\rangle_{eq} = \langle E\rangle_a = 2.44\) (Fig. (a)), and five random initial condition sets (Figs. (a), (b), (c), (d), (e), and (f)) leading to the last metastable state with total energy \(\langle E\rangle_b = 5.23\), \(\langle E\rangle_c = 5.64\), \(\langle E\rangle_d = 6.69\), \(\langle E\rangle_e = 7.09\),
of four parameters. The function $f$ density function $\gamma$.

We fit the above distributions with the probability between the former
creating the overall picture in Fig. $p$.

picky velocity distribution around the amplitudes (higher
energy) with negligible values $p$. The inset in
(a) and (f) present the top of the respective distribution.

and $\langle E \rangle_f = 7.49$, respectively, we determine the normalized
velocity distributions over $10^8$ integration points and present
them in a log-linear scale. As expected, we observe
significant deviations from the Gaussian behaviour when the system is in the metastable state. The Gaussian
symmetry breaks creating new statistics of two symmetric
maxima. More precisely, the higher the energy of the
metastable state is, the more the aforementioned maxima
separate from each other. This is caused by the super-
position of two distinct velocity distribution behaviours.

While the $2N_b$ sites fluctuate around thermal equilibrium
(Gaussian distributions), the "breather-site" acts as an
independent (decoupled) deterministic $φ^4$-oscillator, i.e.,
picky velocity distribution around the amplitudes (higher
picks for higher oscillation energy) with negligible values
between the formers creating the overall picture in Fig. $2$. We fit the above distributions with the probability
density function

$$P(v_N) = \alpha e^{-f(v_N)v_N^2}, \quad f(v_N) := \beta(1 - \delta |v_N|^\varepsilon), \quad (5)$$

of four parameters. The function $f(v_N)$ captures the deviations
from the Gaussian behaviour. The results are
presented in Table II. The parameter $\alpha$ and $\varepsilon$ weakly variate
for the various states keeping very low values confined in the
ranges $0.002 \leq \alpha \leq 0.005$ and $0.1 \leq \varepsilon \leq 0.3$. The latter
exponent shows that $f$ tends to a constant function,
and accordingly the distribution $P(v_N)$ presents Gaussian
characteristics, the more the velocity departs from zero.
Conversely, when it approaches zero its contribution on
$P(v_N)$ becomes essential yielding strong deviations from
gaussianity. The multiplicative factor $\delta$ decreases con-

and $\langle E \rangle_a < \ldots < \langle E \rangle_f$ of the system (see text). The black dashed line is the result of the fitting function in Eq. $5$. The insets in
(a) and (f) present the top of the respective distribution.

| Plot→ | (a) | (b) | (c) | (d) | (e) | (f) |
|-------|-----|-----|-----|-----|-----|-----|
| $α$   | 0.005 | 0.003 | 0.003 | 0.002 | 0.002 | 0.002 |
| $β$   | 505 | -198 | -1230 | -1756 | -1924 | -2027 |
| $δ$   | 0.0 | 4.47 | 1.48 | 1.37 | 1.35 | 1.34 |
| $ε$   | — | 0.3 | 0.1 | 0.1 | 0.1 | 0.1 |
| $χ^2(10^{-2})$ | 1.00 | 1.18 | 2.09 | 2.13 | 1.95 | 2.13 |

TABLE I: Fitting parameters of Eq. 5 for the plotted distributions in Figs. 2(a)-2(f).

Considering higher metastable states varying in the range $4.47 \leq \delta \leq 1.34$. Of course, at equilibrium in Fig. 2(a) its value is by default equal to zero. Last but not least, the parameter $β$ presents a clear distinction between equilibrium and metastability being positive in the former and negative in the latter case. Moreover, the higher the energy of the metastable state is, the lower $β$’s algebraic value becomes making the distribution pickier.

Breather life-time.- We investigate the influence of the coupling constant $k$ on the life-time of a single breather. Therefore, we perform a modified but equivalent version of the relaxation procedure described previously in the following sense. We thermalize the whole lattice at temperature $T_b$ and then, at time $t_0$ we choose randomly one oscillator to which a large amount of extra energy $300 \times \langle E \rangle_{eq}$ is provided to assure that the former excitation corresponds to a breather. At the same time, the dissipation coefficient $γ$ for this particular oscillator is set equal to zero. Then, the time interval $Δt := t_f - t_0$,
where \( t_f \) is the time of reaching again the equipartition energy, defines the desired life-time of the breather. In Fig. 3(a), a representative example of a breather generation according to the preceding procedure and its subsequent decay is recorded. At \( t_0 = 1000 \) we insert energy \( 300 \times \langle E \rangle_{eq} \) into the oscillator at the 25th site, and then let the whole system to reach again thermal equilibrium in order to estimate \( t_f \). In Fig. 3(b), the life-time of a breather, \( \Delta t \), is plotted with respect to the coupling constant \( k \) in a log-log scale for three different temperatures \( T_b \). The final trajectories for each \( T_b \) determining \( \Delta t \) are obtained after averaging over 100 experiments. As can be seen, for all three temperatures, \( \Delta t \) exhibits a power-law behaviour as \( k \) approaches the anticontinuous limit. 

For a qualitative description of the numerical data we fit them with the function

\[
\Delta t(k) = A_i + B_i \ k^{-\lambda_i}. \tag{6}
\]

The \( \{A_i, B_i\} \)-coefficients are determined as \( A_1 = 138.8 \pm 0.05, A_3 = 138.8 \pm 0.05, A_1 = 138.8 \pm 0.05, \ A_3 = 138.8 \pm 0.05, \ B_1 = 0.24 \pm 0.02, B_2 = 4.52 \pm 0.003 \) and \( B_3 = 153.7 \pm 0.02 \) presenting as well as the \( \lambda \)'s, \( \lambda_1 = 2.3 \pm 0.05, \lambda_2 = 2.56 \pm 0.03 \) and \( \lambda_3 = 2.02 \pm 0.03 \), a heat bath temperature dependence. This power-law dependence with the slope lying in the range \( (2,3) \) is a sign of the coherence induced locally by the discrete breathers and self-organization indicating the existence of correlations between the system variables.

Conclusions.- During the energy relaxation process of one-dimensional nonlinear lattices when bringing them in contact with a colder bath of non-zero temperature \( T_b > 0 \), the system may stay for very long times in various metastable states. The decay of the energy of the system with respect to time exhibits a staircase pattern, through a sequence of metastable states, that ends at thermal equilibrium. Considering the metastability of a single breather state we have statistically explored the lattice velocity distribution \( P(v_N) \) observing non-gaussian behaviours. The deviations from gaussianity (thermal equilibrium) has been captured by assuming a velocity dependent factor of the \( v_N^2 \)-term. In the frame of one-breather study we have demonstrated that the lifetime of the former presents a power-law dependence on the nearest-neighbour coupling constant \( k \) when the latter is close to the anticontinuous limit.

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