Intermittent relaxation in hierarchical energy landscapes

A. Fischer[1], P. Sibani[2] and K. H. Hoffmann[1]

[1] *Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany*
[2] *Institut for Fysik og Kemi, SDU, DK-5230 Odense M, Denmark*

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Abstract. - We numerically simulate thermal dynamics in an energy landscape with a hierarchical organization of metastable states. In the model, record sized energy fluctuations are needed to trigger changes from one metastable state to another. The initial configuration is chosen to have a large energy excess, relative to the thermal equilibrium value at the running temperature. We show that the energy surplus trapped in the initial state is dissipated in a series of intermittent bursts, whose rate decreases as the inverse of the age of the system. In addition, one observes energy fluctuations with a zero centered Gaussian distribution. These describe the pseudo equilibrium dynamics within a single metastable state and do not contribute to the energy dissipation. The derivative of the thermal energy with respect to the logarithm of time is asymptotically constant, and comprises a temperature independent part, and a part with an Arrhenius temperature dependence. These findings closely mirror the behavior observed in recent numerical simulation of microscopic glassy systems, showing that the simple assumptions built into the present model are sufficient to explain the phenomenology.

Introduction. – Many characteristic features of low temperature glassy dynamics are only weakly related to details of the microscopic interactions. Aging processes, for example, generically follow a change of an external parameter, e.g. a temperature quench. In *mesoscopic* sized samples [1, 2] a sequence of large, so-called intermittent, configurational re-arrangements is observed. These fluctuations have an anomalously large size and generate non-Gaussian tails in the probability density function (PDF) of configurational probes such as colloidal particle displacement [3, 4] and correlation [5] or voltage noise fluctuations in glasses [6]. In different model systems [7, 8], the Probability Density Function (PDF) of the energy fluctuations following a thermal quench features a zero centered, equilibrium like Gaussian and an exponential tail which covers large negative changes. The latter is related to shifts between different metastable attractors. Based on the idea that the attractors dynamically selected during the aging process are marginally stable [9, 10], the so-called *record dynamics* scenario [7, 10] links the intermittent events, or *quakes*, to record-sized energy fluctuations within thermalized domains of the system.

Record fluctuations are characterized by their rank, but do not possess a definite scale. For this reason alone, they will not produce observable effects, unless the energy landscape supporting the fluctuations is self-similar under a change of energy scale. Within a self-similar energy landscape, record sized fluctuations are required to induce attractor changes. These typically lead the system from shallow attractors typically selected by the initial quench into gradually more stable attractors [10]. A hierarchy of energy and/or time scales is a simple mesoscopic model description of energy landscapes [11–15], which can nonetheless explain many facets of complex relaxation [13, 16–18]. A simple incarnation of this idea is thermal hopping in a tree structure: The nodes of the tree stand for lumped sets of microscopic configurations. Beside their connectivity, the nodes are characterized by an energy and a degeneracy. A specific example, the so-called LS tree model [18, 19] has inequivalent energy minima, which belong to different subtrees and thus label different metastable configurations. The model's scale invariance is restricted due to finiteness of the elementary energy scales L and S. The statistics of the quakes in a record dynamics description would only be exact in the limit where L and S vanish, while the energy difference between the lowest and the highest energy level remains constant.

To minimize the unwanted effects of finite energy scales, the present study considers a randomized LS tree model. While exact analytical results are no longer possible, the

model still offers a strikingly simple and general conceptualization of a highly complex relaxation behavior.

In this Letter, energy traces are obtained from isothermal simulations of an ensemble of randomized LS model aging after a quench. The energy fluctuations are treated as experimental time-resolved calorimetry data. The probability density function (PDF) of the energy fluctuations shows, as expected, the fingerprints of intermittent heat flow. The form of the local density of states of the attractors is extracted form the Gaussian part of the fluctuations, and the rate of energy flow is extracted from the tail. To validate the method of analysis, the information is compared with the known properties of the model.

Modified LS-tree ensembles. – The randomized LS model used in the simulations can be pictured as an upward rooted tree with the vertical scale representing the energy. The n'th level of the tree comprises all the nodes connected to the root by precisely n edges, with $n = 0, \ldots, N$. With the exception of the 'bottom' level with index $n = N$, each node is connected to two 'daughters' of lower energy by a 'Longer' and a 'Shorter' edge. The modification of the original model [18] consists in choosing, independently for each level, new random values of L and S, as discussed further below. Accordingly, the energy differences along the 'Longer' and 'Shorter' edges are $\Delta E = L_n$ and $\Delta E = S_n$ for each level n. The above procedure removes the oscillation on a logarithmic timescale characteristic of a regular tree, concomitantly decreasing the energy scale corresponding to the smallest barrier in the system. Each node represent a lumped set of configurations and hence possesses a degeneracy. In the model, the degeneracy of a node equals that of its L_n and S_n daughters, multiplied by a factor κ_{L_n} and $\kappa_{S_n} \leq \kappa_{L_n}$, respectively. Bottom nodes are not degenerate. With this prescription, the overall degeneracy of the model increases in a nearly exponential fashion, as the level index increases from a bottom node. A list of values

$$\mathcal{E} = \left\{ 2^{\frac{i}{4}-1} \ : \ i = 0 \ldots 19 \right\} \quad . \tag{1}$$

describes the possible energy differences. For each level of the tree, two values are drawn independently and with uniform probability from the list. They may be equal, and they are assigned to L and S such that $L \geq S$.

Thermal relaxation is modeled as hopping between neighboring nodes, with up and down rates defined by:

$$\Gamma_{\mathrm{up},j} = f_j \kappa_j \mathrm{e}^{-\beta \Delta E_j} \qquad \Gamma_{\mathrm{down},j} = f_j \ , \tag{2}$$

where the index $j \in \{L_n, S_n\}$ labels L- and S-edges at level n. The hopping rates obey the detailed balance condition $\Gamma(x,y)P_{\mathrm{eq}}(y) = \Gamma(y,x)P_{\mathrm{eq}}(x)$, where the equilibrium distribution is the Boltzmann distribution. So-called kinetic factors f_j are introduced to control the relaxation rate along each edge. Factors independent of j entail a trivial rescaling of the (arbitrary) time unit. In contrast, non-uniform factors considerably modify the dynamics on short time scales after a thermal quench [20]. E.g. choosing $f_{S_n} \gg f_{L_n}$ favors downward transitions along the S edges, ensuring that an initial quench from the top node preferably ends near the shallowest metastable minimum. We achieve the same in a more ad hoc fashion, by choosing the highest lying and most shallow local energy minimum as the initial state for the aging dynamics.

In spatially extended systems with short range interactions, one expects thermalization to occur independently within a number of slowly growing domains or clusters of neighboring degrees of freedom. The configuration space of the full systems correspondingly factorizes into a product of configuration spaces, each term belonging to a single domain. Domains are expected to have a hierarchical organization, which, in the present context, is rendered by a modified LS tree. Accordingly, we consider an ensemble of trees, whose parameters are generated, as mentioned, from the list given in (1).

The dynamics. – The dynamical evolution of a single tree is studied using a rejectionless continuous time Monte Carlo Method [21], which operates with an intrinsic time variable t, initially set to zero. The following three steps are iterated: for the current node, the possible transitions[1] according to (2) are considered. Among those, a choice is made with probability equal to the corresponding transition rate divided by the sum of all rates out of the current node. A random waiting time is then drawn from an exponential distribution with average equal to the reciprocal of the transition rate. This waiting time is then added to the global time. Finally, the transition is effectuated by moving the walker to the corresponding neighboring node.

Each tree in the ensemble is updated independently according to the above rejectionless algorithm. The result is an ensemble of time series, each describing the history of energy fluctuations of one member of the ensemble. The time series describing the total energy of the tree ensemble is then obtained by interweaving the time series into a single data stream ordered by increasing values of the time variable.

In the following, the symbol t stands for the system age, i.e. the time elapsed since the beginning of the simulation. The symbol t_w is the age of the system when data collection for the fluctuation PDF begins. Energy fluctuations are energy differences over a time interval $\delta t \ll t_w$.

Energy Transfer Statistics. – Our results are based on an ensemble of 2000 trees of height $N = 12$, with 5000 independent runs on each tree. The model is set up with degeneracy growth parameters $\kappa_L = \kappa_S = 2.20$ and kinetic factors $f_L = 0.25$ and $f_S = 1.00$. The data pertain to systems initially quenched into the shallowest of the available minima, i.e. the minimum connected to the top node by a series of S links.

[1] In general on upward and two downward transitions are available, except for the bottom states and the top state, which have no downward, respectively upward transitions.

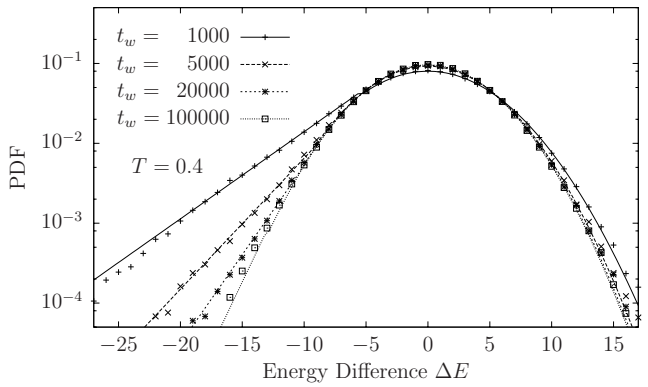

Fig. 1: The PDF of the amounts of energy exchanged between system and thermal bath within the time $\delta t = 100$. Negative values represent an energy outflow, while positive values represent an energy inflow. The data are taken for four logarithmic equidistant times in the interval $t = [10^3 \dots 10^6]$.

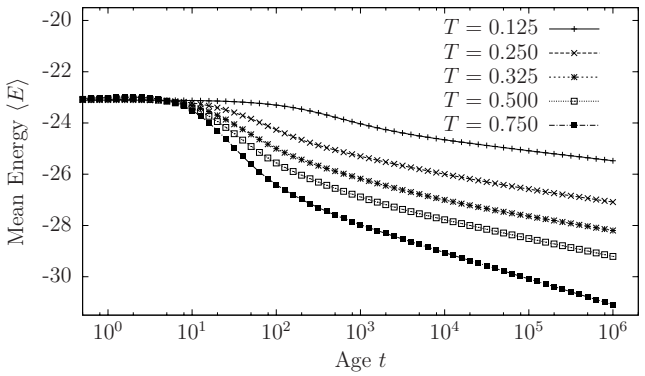

Fig. 2: The mean inner Energy E of the tree ensemble plotted versus system age for different temperatures showing the progress of the relaxation process. Note that after some kind of startup phase lasting until $t \approx 200$ the energy shows a practically straight decrease at logarithmic time scale.

The probability density function (PDF) of the amount of energy exchanged within a time interval δt at a particular system age t

$$H = E(t + k\,\delta t) - E(t + (k-1)\,\delta t) \ . \tag{3}$$

is collected over $k = 1 \dots 100$ time intervals using $\delta t = 1$ and starting at different values of t_w, in the range $10^3 \dots 10^5$. The zero centered Gaussian peak, flanked on the left by an exponential tail seen in figure 1 is the characteristic signature of intermittency. When k and δt are kept fixed, the relative weight of the intermittent tail decreases with increasing t_w. The width of the Gaussian fluctuations is independent of k and δt.

We can then conclude that the fluctuations themselves are uncorrelated for the studied δt and that they describe (pseudo) equilibrium energy fluctuations within partially equilibrated subtrees. Clearly, as the Gaussian fluctuations do not contribute to the net energy flow, the latter is only due to the intermittent events.

The decay of the average energy is shown in figure 2: After an initial transient stretching to approximately $t = 200$, the energy decreases in time in a simple logarithmic fashion:

$$E(t, T) = -a(T)\ \ln(t) + \mathcal{C} \ . \tag{4}$$

In this model, a quake occurs when the lowest value of the energy seen in the simulation decreases. This corresponds to a first visit to a new subtree containing states of lower energy. The logarithmic rate of the energy loss $a(T)$, is the product of the rate of quakes and the average amount of energy released in a single quake. The temperature dependent offset $\mathcal{C}$ is related to the initial stage of the relaxation and has no importance for our treatment. A clear sign of the non-equilibrium nature of the dynamics, also observed in microscopic models [22], is that the thermal energy reached at a fixed time is higher the lower the temperature. According to (4) the rate of energy loss $r_E = -\mathrm{d}E/\mathrm{d}t$ has the form

$$r_E(t) = -\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{a(T)}{t} \ , \tag{5}$$

which fully agrees with the numerical results shown in figure 3 as well as with similar results for microscopic model simulations [7, 22]. The figure depicts the rate of energy loss for selected temperatures (symbols) together with lines according to (5).

Figure 4 shows that the Arrhenius form $\log(a(T) - 0.195) = b/T + c$ provides an reasonable description of the logarithmic rate of energy loss, $a(T)$. The shift in the value of $a(T)$ was obtained by an educated guess judged to provide the best agreement with the Arrhenius form. The parameters b and c where then estimated by least square fitting. The value of the 'barrier' parameter $b = -0.307$ is close to the value of the smallest energy barrier present in the model, $b_{min} = 0.5$.

Figure 5 shows the bandwidth of the Gaussian fluctuation σ_{rev} versus the temperature. The curve is relatively featureless and increases with temperature as expected. For a classical system (with constant heat capacity) the fluctuation bandwidth would be proportional to T. The data shown have a slightly faster than linear increase with T.

Discussion and conclusion. – Hierarchical tree like models are very good prototypes for studying relaxation phenomena on energy landscapes [16, 19, 23–32].The hierarchical model studied in this Letter is a modification of the even simpler LS model [19], which has nonetheless glassy features like rejuvenation and memory effects [18]. The modification replaces the two elementary energy scales of the LS model with a wider spectrum, in order to remove unphysical logarithmic oscillations [12] which would affect the energy relaxation behavior.

We have observed that the intermittent energy relaxation of the model has statistical properties very similar to those observed in microscopic models [7, 22] and,

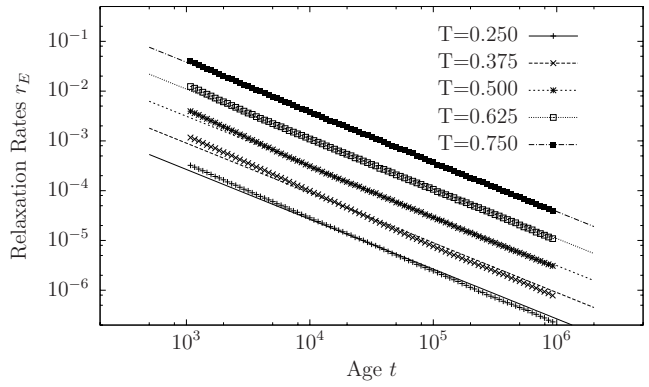

Fig. 3: The rate of energy loss r_E is plotted versus system age for different temperatures. The lines have the form $r_E = a(T)/t$ with the constant a as in equations (4) and (5). To avoid clutter, the data set for each T is multiplied by 1, 3, 9, ... in order of increasing T. A similar but much smaller shift of the curves in the same direction is present due to the temperature dependence of a.

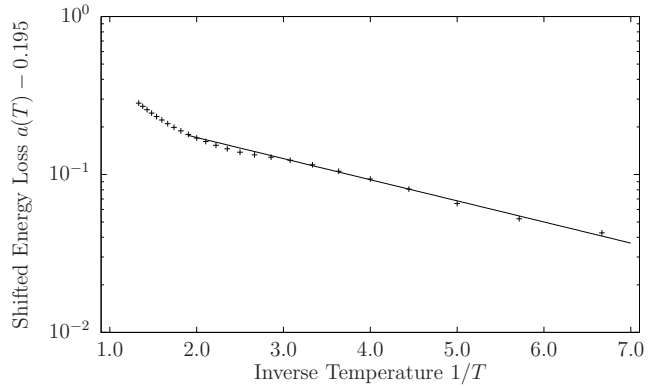

Fig. 4: The logarithmic rate of energy loss $a(T)$ (see (5)), shifted by 0.195, is plotted vs. the inverse temperature. The data are fitted to the expression $\log(a(T)-s) = b/T+c$ yielding $s = 0.195$, $b = -0.307$ and $c = -1.147$.

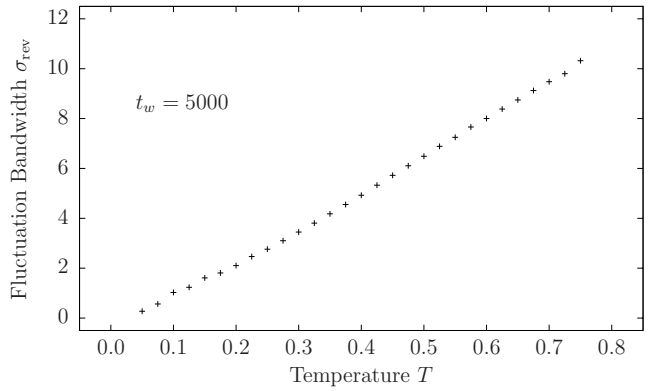

Fig. 5: The standard deviation of $\sigma_{\rm rev}$ plotted versus temperature is obtained from the gaussian part of the energy exchange PDF.

for quantities other than the energy, also in experimental systems [2, 33]. The behavior can be understood as follows: At any given time, the probability distribution of the model is supported within a finite subtree. Assuming that this distribution is equilibrium-like [17], i.e. neglecting the transient regime pertaining to the local equilibration process, a larger subtree must be entered in order to lower the hitherto lowest energy. This entails overcoming an energy barrier larger than the largest barrier currently overcome. In other words, a record sized energy fluctuation is necessary (but not sufficient) to reach a lower energy state. The exact same feature has been observed in the Edwards-Anderson spin-glass, with thermal hopping [34] as well as extremal optimization [35] used as update rules. Summarizing, record-sized energy fluctuations trigger, with a certain probability, quakes which then lead to the attainment of lower energies. Since the records occur at a rate proportional to $1/t$ [9], the rate of quakes is also proportional to $1/t$ and the quantity $r_E \times t = -a(T)$ is, modulo a constant proportionality factor, the energy given off in a single quake.

Within a hierarchical model, the origin of the behavior is, by construction, that record sized energy fluctuations are needed to move the system from one metastable region of configuration space to a different metastable region with a lower energy. We have shown that this property suffices to generate realistic spectra for the intermittent energy fluctuations.

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