The energy landscape of aging systems—from a different angle

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Abstract. – A novel method for glassy landscape exploration is presented which utilizes a time series of energy values collected during an isothermal relaxation after a thermal quench. A sub-series of increasingly rare events, or quakes, which are connected to an irreversible release of energy from the system, is used to identify entry and exit times for landscape valleys. The landscape of three dimensional spin glasses is studied from this angle for a number of lattice sizes and for a range of low temperatures. A simple picture emerges regarding the temperature and size dependence of (1) the energy barriers separating the valleys, (2) the lowest energy minimum within a valley, and (3) the distance between the configurations belonging to the lowest minima in neighboring valleys. The configuration changes following the quakes are analyzed in terms of connected clusters of flipped spins, and the size distribution of these clusters is presented.

Introduction. – Macroscopic properties of thermalizing glassy systems depend on the time (age) elapsed after the quench into the glass phase: on time scales shorter than the age, pseudo thermal equilibrium establishes itself locally within metastable regions of the landscape while on longer observational time scales the relaxation is manifestly non-stationary [1,2,3]. Memory and rejuvenation effects resembling those observed in spin glasses [4] are also present in e.g. microscopic models of driven dissipative systems [5], where they are related to an irreversible dynamical selection of marginally stable attractors [6,7,5]. This suggests that similar mechanisms could be present in thermal aging as well.

To discuss the connection between aging and landscape geometry it is crucial (i) to identify the dynamical events, or ‘quakes’, marking the transition between equilibrium and non-equilibrium dynamics, and (ii) to characterize in configuration and/or real space the attractors, or ‘valleys’ dynamically selected by these quakes. The approach developed below strives to guarantee the dynamical relevance of the structures identified (minima, barriers, etc.) by solely relying on a statistical analysis of time series collected during unperturbed aging following an initial quench. Our method is generally applicable to glassy systems and can, with a small computational overhead, complement established landscape mapping procedures such as e.g. the Stillinger-Weber approach [8,9,10,11,12,13], which employ e.g. thermal quenches to study local energy minima.

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The method is demonstrated by an application to short range spin glasses, mainly nearest neighbor models on three dimensional cubic lattices. Our results concern the energy barriers which are surmounted by the quakes, the frozen-in energy they release, and the corresponding configurational rearrangements.

![Fig. 1](image1.png)

**Fig. 1** – A fictitious time series of collected energy values illustrates our sampling procedure and our definition of a valley (= gray area). Conspicuous events, i.e. energy and barrier records, are denoted by circles and squares. The black squares indicate the entry and exit time in the valley, while the black circles show the lowest energy record which allegedly corresponds to an energy minimum.

![Fig. 2](image2.png)

**Fig. 2** – Main figure: the average number $n_v$ of valleys visited in the time interval $[0, t]$ is plotted versus time. The data pertain to 3d gaussian spin glasses of size $N = L^3$. Insert: the corresponding logarithmic slopes of $n_v$ as a function of the logarithm of the system size $N$. These data are nearly insensitive to temperature or system type: Triangles: 2d, $T = 0.4$. Circles: 3d, $T = 0.5$.

**Method.** – The idea that progressively deeper and more stable attractors are explored during aging appears in different guises in a number of mesoscopic models [14, 15, 16, 17, 18, 19, 20] which can reproduce many aspects of aging phenomenology. Implicit in that sort of modeling is a temporal sequence of increasingly rare non-equilibrium events each overcoming a dynamical barrier higher than all those previously surmounted.

To investigate the occurrence of such events in the actual dynamics of microscopic models, it is natural to look at extremal values of the energy in the data stream produced by a simulation: We keep track of the current lowest energy encountered, $E$, and of the current highest barrier $B$ overcome. With a slight abuse of notation, a barrier is simply the energy of the current state measured from $E$, and, as such, does not necessarily provide access to new regions of configuration space. Henceforth, $E$ and $B$ will be referred to as energy and barrier records.

Whenever a system is locally equilibrated at low $T$, the current state of lowest energy is likely to be repeatedly visited by the (recurrent) fluctuations. By this token, the appearance of a lower $E$ value implies that local equilibrium is broken. Once a trajectory is headed downhill, an entire sequence of $E$, corresponding to transient configurations, may arise which is unrelated to landscape minima. Only the $E$ value preceding a barrier record has potential physical significance, since it will again be repeatedly visited and is likely associated to a new local equilibrium situation. Similarly, the sequence of barrier records of roughly the same magnitude which may appear while a trajectory crosses high ‘saddles’ is uninteresting, except
for the highest barrier record preceding a new low energy minimum.

Consider now a sequence of energy and barrier records, e.g. the $EBBEBBEBE$ shown in Fig. 1. As argued, we only keep the full squares and circles (the ‘⊗’ symbol represents a datum removed) thereby reducing our string to its final state: $E(BEB)E$. Within the triplet $(BEB)$ the two $B$’s identify, by definition, the entry and exit times of a valley, and the $E$ identifies the time $t_{hit}$ at which the lowest state of the valley is hit for the first time. The recurrent quasi-equilibrium fluctuation regime starts at $t_{hit}$ and lasts until the valley is exited. Energy minima which are not records are not assigned a separate valley, and will create an internal structures within each valley. Finally, no new valleys can ever appear after the ground state is discovered.

Our protocol is maximally restrictive in its definition of a new valley: different landscape minima are lumped together whenever either they or the energy barriers separating them are degenerate. Even models whose aging purely originates from entropic sources [21] would only produce one valley. In the spin glass energy landscape the approach nonetheless uncovers a great deal of structure, whose dynamical significance is more fully discussed in Refs. [22, 23].

For simulation speed, we rely on the Waiting Time Method (WTM), a rejectionless Monte Carlo scheme [24] well suited for problems where $N$ variables contribute additively to the energy through local interactions. Based on the local field, each variable is stochastically assigned a flipping time and the variable with the shortest flipping time is updated together with the local fields affected by the move. The sequence of WTM moves equals in probability [24] the sequence of accepted moves in the Metropolis algorithm. The current flipping time, henceforth simply ‘time’, corresponds to Metropolis sweeps, as well as to the physical time of an experiment.

**Model.** We consider $N$ Ising spins interacting via the Edwards-Anderson Hamiltonian [25]

$$\mathcal{H}(\alpha) = -\frac{1}{2} \sum_{i,j} J_{ij} s_i^{(\alpha)} s_j^{(\alpha)}. \tag{1}$$

In this formula, $s_i^{(\alpha)}$ is the spin value at site $i$ for configuration $\alpha$, the couplings $J_{ij}$ are symmetric in their two indices and vanish unless $i$ and $j$ belong to neighboring sites. In the latter case they are drawn independently from a Gaussian distribution of unit variance. We mainly consider regular lattices of linear extension $L$ in three dimensions, where $N = L^3$. The dynamics is single spin flip with detailed balance.

**Results.** To obtain meaningful comparisons, all data originating from the first ten time units after the quench were discarded. Secondly, the index identifying each valley within the ordered sequence of valleys visited—for short valley index—was shifted up to two units in Figs. 3 and 4. Unless otherwise specified, our data are quenched averages over an ensemble, whose size varies from 30000 for the smallest systems to 4000 for the largest ones. In all cases, the amount of statistics was sufficient to remove any visible scatter. The systematic error left stems from the finite run time coupled to the broadness of the distribution of the intervals between successive quakes. This leads to a considerable variation in the number of valleys seen in different runs. Data corresponding to valley indices achieved by less than 75% of the ensemble were discarded to reduce the error.

A basic quantity is the average number $\langle n_V(t) \rangle$ of quakes or valleys plotted in Fig. 2 as a function of $\ln t$. Note that the smooth appearance of the curves stems from the large amount of data available, rather than from fitting. All the plots in the main figure belong to $3d$ systems of growing size, while similar data in $2d$ and for smaller systems were omitted for clarity. The insert shows the logarithmic rate of events $\alpha = d \langle n_V(t) \rangle / d \ln t$, in $2d$ as well as $3d$, as a function
Fig. 3 – The average size of the barrier $B$ separating contiguous valleys in 3d spin glass landscapes is scaled with $L$ and $T$ as indicated in the ordinate label and plotted versus the valley index $n$. The combinations of $L$ and $T$ values specified in the figure were included in the scaling plot. The abscissa pertaining to different data sets is shifted by amounts of order one.

Fig. 4 – The average difference $\Delta$ between the lowest energies of the first valley and the $n$’th valley is plotted versus the valley index $n$. The ordinate is scaled with $L$ as indicated, and the abscissa pertaining to different data sets is shifted by amounts of order one. The small $T$ dependence of $\Delta$ implies that nearly the same energy is lost through $n$ quakes at different temperatures, even though the barriers overcome widely differ.

of $N = L^d$. The derivative was calculated, ignoring the small systematic curvature, as the average slope between times $10^4$ and $10^6$. Notably, $\alpha$ is highly insensitive to the temperature, and to the system dimension. The variance of $n_V$ was also calculated and its ratio to the average found to be constant, except at short times. These properties are accounted for by a log-Poisson statistical description [7], whose connection to glassy dynamics is developed in Ref. [22].

The statistics implies that the energy function decorrelates between consecutive quakes. Since the correlation time and relaxation time (for the internal thermalization) can be generically identified [29], quasi-equilibrium is typically achieved before the valley is exited.

Conversely, whenever dynamical trajectories dwell near a local minimum, record high energy fluctuations decorrelate, and, hence, a log-Poisson distribution applies to them [7]. Crucially, the definition of a quake additionally requires the achievement of a record low energy value. The availability of such minima mirrors the landscape geometry and the selection of the initial attractor. E.g., if the trajectories were started at the ground state, the system would for ever remain in the same valley. The fact that the same statistical description covers barrier records as well as quakes shows that climbing the former triggers the latter. The logarithmic rate of events grows with the lattice size $N$ as shown in the insert of Fig. 2, i.e. in a nearly logarithmic fashion, from an initial value close to 1 to a value close to 2 for extremely large system sizes. For a Poisson process this rate is proportional to the number of lattice ‘regions’ evolving independently [22], and its reciprocal is therefore proportional to the size in real space of the region affected by a quake. Importantly, the logarithmic nature of the statistics implies that the time spent to reach the bottom of a valley entered at a time $t_w$ is proportional to $t_w$ [22], whence the near-extensive configurational and energy changes we observe are not the outcome of instantaneous processes.
Further insight into the properties of quakes can be gained through the scalings shown in Figs. 3 and 4. Figure 3 describes the scaling with $L$ and $T$ of the average energy barrier $B$ separating two contiguous valleys, while Fig. 4 depicts the average difference $\Delta(1, n) = E_1 - E_n$ between the state of lowest energy in valleys 1 and $n$. While we have not attempted a quantitative determination of the uncertainty on the scaling exponents, changing the last significant digit visibly affects the quality of the collapse.

The smooth and nearly linear increase of the energy barrier with $n$ confirms the expectation that the valleys gradually become more stable against thermal fluctuations. The growth of the barriers with system size is $\propto L^{1.16}$, while the typical range of the energy fluctuations is $\propto L^{3/2}$. While the slower growth observed is consistent with a bias favoring low energy saddles, the strong temperature dependence $\propto T^{1.8}$ clearly indicates an entropic effect: A linear $T$ scaling would apply if the saddle of lowest energy were the only route utilized. The average Hamming distance $H_d$ between the bottom states of contiguous valleys (see Ref. 23 for a figure) was also investigated and found to scale with $L^{2.85}$ and $T^{1.70}$.

Turning to Fig. 4, the initially linear increase of $\Delta(1, n)$ is seen to slowly taper off, possibly reflecting a change in landscape geometry closer to the ground state. The $L^{2.65}$ dependence of $\Delta(1, n)$ also characterizes its derivative with respect to $n$, i.e. the energy difference $\Delta(n, n+1)$ between neighbor valleys.

The weak temperature dependence of the scaling plot is to be contrasted with the strong $T$ dependence of both the barriers overcome and of the Hamming distance. After $n$ quakes, two systems relaxing at different temperatures lose nearly the same amount of energy, even though the configurations visited and the energy barriers crossed substantially differ. Firstly, this implies a strong degeneracy of the minima. Secondly, in conjunction with the striking insensitivity to the temperature of the time statistics of the quakes 22, 23, it implies that the dominant paths at different $T$ widely differ. Qualitatively, this idea appeared early in the spin-glass literature 27, and was later incorporated in a model 15 showing rejuvenation effects 4. In a broad sense, our findings concur with the view of aging as activated dynamics within a hierarchy of energy barriers 14, 15, 16, 17, 19, 20.

As shown in Fig. 5, spins flipped through a quake fall into $m$ connected clusters, whose surface carries the corresponding non-equilibrium energy release(1). Letting $n(i)$ denote the number of clusters of size $i$ within a given system and $p(i) = n(i)/m$, we average $p(i)$ over 1000 realizations of the couplings $J_{ij}$ to obtain the distribution of cluster sizes shown in Fig. 4 for a series of quake indices $n$. As a guide to the eye, straight lines are included, representing power-laws with exponents $-2$ and $-3$. As the system ages, the cluster size distribution broadens, with the early decay close to the $i^{-2}$, and with the the tail of the distributions falling off more slowly than $i^{-3}$, except for small $n$. This means that the variance of the cluster size is dominated by the end of the integration interval and thus grows with $N$. Regardless of whether the average cluster size might remain finite or not in the limit of large $n$ and large $N$, the average cluster is never the typical one. As Fig. 6 more than suggests, the latter diverges with the system size. Also note that, were this not the case, the size dependence of the energy and configuration changes $\Delta(n, n+1)$ and $H_d(n)$ would both scale with the number of clusters present in the system. $\Delta$ and $H_d$ would then possess identical $N$ scalings, which contradicts our previous findings.

A direct study of the size dependence of the distribution including even larger sizes is exceedingly difficult to carry out. In order to avoid comparing a larger but younger system with one which is smaller but older, the quake index $n$ must be increased logarithmically as $N$ increases, see e.g. Fig. 2.

(1) Quite unlike droplets 22, 33, which carry the energy accumulated through a quasi-equilibrium fluctuation.
Fig. 5 – The spins overturned by the $n$‘th quake are shown in white in the projection of the two lowest-lying states of valleys $n$ and $n + 1$ onto each other. The data pertain to a $2d$ system of size $N = 50^2$ at $T = 0.3$, with $n = 21$.

Fig. 6 – The distribution of cluster sizes for a $3d$ system of linear size $L = 30$ is shown for a sequence of valley indices $n$. The simulation temperature is $T = 0.4$. The straight lines corresponding to power laws are included as a guide to the eye.

**Conclusions and outlook.** – The gist of our approach is to uncover the dominant structural landscape features, e.g. barriers, minima and distances, as they appear to the unperturbed aging dynamics far from the ground state and far from global thermal equilibrium. We strongly emphasize the qualitative difference between local equilibrium fluctuation dynamics within a valley and the non-equilibrium quake dynamics through which the energy trapped by the initial quench is slowly released. The latter process, which is practically irreversible on the time scales considered, has not received much theoretical attention. A recent effort [22] describes it in terms of a log-Poisson process, establishing a connection to driven dissipative dynamics [7, 5] and evolution models [28, 29], where the pace of the dynamics similarly decelerates while the system ages.

Uniquely to our landscape approach, the resolution of the probe self-adjusts to detect gradually coarser scales as the pace of the dynamics slows down. The picture with emerges confirms the presence of a hierarchy of dynamical barriers which must be overcome in order for the system to relax, and complements the results obtained by other methods. In the diffusive dynamics of atomistic glassy models above the glass transition temperature studied by Doliwa and Heuer [13], energy barriers also play a decisive role, and ‘metastructures’, which similarly to our valleys comprise many local minima labeled by their lowest energy state, are the main objects in a coarse grained dynamical description. In short range spin-glasses, the morphology of local energy minima with energy of order one relative to the ground state was investigated by Krzakala, Martin and Houdayer [30, 31]. These states differ from the ground state on a set of spins spanning the whole system, which clearly separates them from droplet-like excitations and suggests a similarity to the quake-induced rearrangements shown in Fig. 4. Clearly, the dynamical regime presently considered remains quite far from the ground state, and the energy difference are also far being of order one. In the extreme asymptotic regime where quakes become increasingly rare even on a logarithmic time scale—a trend visible for small systems in Fig. 1—the energy released must however approach zero. If the trend expressed by Fig. 5
continues in this regime, our dynamically identified clusters might then have morphological properties similar to the 'sponges' in Refs. [30, 31].

Let us finally consider the connection to pseudo-equilibrium thermal correlations [34]. In short-ranged spin-glasses these are established on an age dependent length scale \( l(t_w) \) which can be extracted from a four point thermal correlation function. This scale i) grows in a slow power-law fashion with the age of the system, and ii) stays below \( l(t_w) \approx 4 \) in the range of temperature and times presently considered. Since four point correlations are insensitive to a coherent spin flip occurring on a scale much larger than \( l(t_w) \), and since equilibrated clusters or droplets easily fit inside the much larger quake-induced rearrangements implied by Fig. 6, the non-equilibrium de-excitation mechanism presently described seems only weakly, if at all, coupled to the local thermalization process. This is completely in line with the approach of Ref. [22].

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