Real space analysis of inherent structures

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Abstract. – We study a generalization of the one-dimensional disordered Potts model, which exhibits glassy properties at low temperature. The real space properties of inherent structures visited dynamically are analyzed through a decomposition into domains over which the energy is minimized. The size of these domains is distributed exponentially, defining a characteristic length scale which grows in equilibrium when lowering temperature, as well as in the aging regime at a given temperature. In the low temperature limit, this length can be interpreted as the distance between ‘excited’ domains within the inherent structures.

A significant part of our understanding of the low temperature behavior of disordered systems comes from the landscape picture, which was first introduced as a free-energy landscape, in the context of mean-field spin-glasses [1–3] –yet more qualitative landscape ideas for structural glasses appeared earlier [4]. A complementary approach, more suitable for numerical simulations, is to consider the potential energy (instead of free-energy) landscape, which relies on the notion of inherent structure (IS). These IS are defined as local minima of the potential energy in phase space, i.e. they are stable against a set of elementary transitions defined by the dynamical rules. This notion has been shown to be very useful for the understanding of glassy dynamics, both in disordered [5–7] and non disordered systems [8, 9].

On the other hand, many efforts have also been devoted to the understanding of the real space properties of disordered systems. This includes in particular the structure of low energy excitations over the ground state [10,11], as well as the identification of a correlation length through the definition of a four-point correlation function, which compares the dynamical state of two copies of the system having the same disorder, but independent thermal histories [12–16]. By definition, the length scale deduced from this four-point correlation function characterizes the current configuration visited dynamically by the system. Yet, since IS are believed to play an important rôle in the dynamics of disordered systems, one may wonder whether there also exists a length scale characterizing the underlying IS. A few examples of spatial analysis of IS have been known for long –see e.g. [17] for the disordered Ising chain– but this analysis was considered as a technical procedure to compute the configurational entropy rather than a way to introduce a characteristic length scale. Besides, the issue of characteristic length scales for IS was addressed recently in the context of kinetically constrained...
models (models with no interactions, but with kinetic constraints), where IS are found to differ from the ground state only by a set of local defects \[18\]. Still, in systems with more complex hamiltonians than kinetically constrained models, including for instance disordered interactions between sites, the spatial structure of IS essentially remains an open issue.

In this Letter, we show within the context of a simple disordered model that IS exhibit a non trivial real space structure. A numerical algorithm allows us to decompose explicitly an IS into essentially non-overlapping ‘regions’ upon which the IS identifies with an absolute energy minimum. The size of these regions is found to be distributed exponentially, leading unambiguously to a characteristic length scale $\xi^*$, which grows in the aging regime before saturating to an equilibrium value that increases when lowering temperature. An interpretation in terms of small excited domains in the low temperature limit is also proposed.

**Model and thermodynamics.** – The model we introduce below is aimed at being a simplified coarse-grained description of disordered systems. For simplicity, only the one-dimensional case is considered in the following. We assume that space is divided into cells, labeled by an index $i = 1 \ldots N$, and that the internal state of the system within each cell can be described by a variable $q_i$ taking integer values between 1 and $M$. The set of variables $\{q_i\}$ is denoted by $q$ in the following. To account for the interactions between neighbouring cells, we introduce an interaction energy $V_{i,i+1}(q_i,q_{i+1})$, which a priori takes different values for each couple of variables $(q_i, q_{i+1})$, and for each link $(i, i+1)$. To be more specific, the interaction terms $V_{i,i+1}(q_i,q_{i+1})$ are independent quenched random variables drawn from a distribution $\rho(V)$ for each link and for each value of $(q_i, q_{i+1})$; note that $V_{i,i+1}(q,q') \neq V_{i,i+1}(q',q)$. The hamiltonian is defined by $H = -\sum_{i=1}^{N} V_{i,i+1}(q_i,q_{i+1})$, with periodic boundary conditions. This model can be thought of as a generalization of the disordered Potts model. In the latter one assumes that $V_{i,i+1}(q_i,q_{i+1})$ can take only two distinct values, one for $q_i = q_{i+1}$ and the other for $q_i \neq q_{i+1}$. In the present model, $V_{i,i+1}(q_i,q_{i+1})$ takes $M^2$ distinct values, as in the physical picture described above, there is no reason why the interaction energies should be equal for different values of $(q_i,q_{i+1})$.

In the following, we restrict ourselves to the case of an exponential distribution $\rho(V) = V_0^{-1}e^{-V/V_0}$; $V_0$ is set to unity in the following. We have studied the thermodynamic properties
of this model, namely the free energy density $F(T)$ and the entropy density $S(T)$. The canonical partition function is obtained by computing numerically the product of transfer matrices, which allows to reach system sizes as large as $N = 10^5$. The entropy $S(T)$ is plotted on Fig. 2(a) for different values of $M$; one sees that the entropy remains regular when $T \to 0$.

Aging properties. – Turning to dynamics, one needs first to define the kinetic rules according to which the system evolves. We use a one-site Glauber dynamics at temperature $T_i$, with a transition rate associated to site $i$, $W_i(q \to q') = \tau_0^{-1}/[1 + \exp(\Delta U_i/T)]$, where $\Delta U_i = U_i(q') - U_i(q)$. The microscopic time scale $\tau_0$ is taken as the time unit in the following. The local energy $U_i(q)$ is the sum of the interaction terms with the neighbors of site $i$, $U_i(q) = V_{i-1,i}(q_{i-1}, q_i) + V_{i,i+1}(q_i, q_{i+1})$.

So as to give evidence for the aging dynamics that takes place at low temperature before the system equilibrates, we introduce a simple correlation function $C(t_w, t_w + t)$ defined as the average overlap between configurations occupied at time $t_w$ and $t_w + t$:

$$C(t_w, t_w + t) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \delta_{q_i(t_w), q_i(t_w + t)} \right\rangle$$

where the brackets $\langle \ldots \rangle$ denote an average over the thermal histories. Numerical results are shown in the left inset of Fig. 2(b) for different waiting times $t_w$, starting from an infinite temperature initial condition. The correlation $C(t_w, t_w + t)$ clearly exhibits aging properties, as the relaxation time depends strongly on $t_w$. The same data are shown in the main plot as a function of the rescaled time $t/t_w$, showing a good collapse at least in the considered time window. For times $t$ larger than the equilibrium relaxation time $\tau(T)$, aging becomes interrupted; $\tau(T)$ is seen to increase according to an Arrhenius law, $\ln(\tau(T)) \sim 1/T$ – right inset of Fig. 2(b).

Inherent structures and spatial analysis. – An inherent structure (IS) is defined as a configuration of the system from which the global energy cannot be lowered by changing the state of a single site. A deterministic algorithm allows to associate unambiguously an IS to any instantaneous configuration: starting from this configuration, one looks at each step for the one-site transition that lowers as much as possible the global energy. The procedure is
iterated until an IS is reached, and the corresponding configuration \( \{ q^\text{IS}_j \} \) is recorded. This algorithm is close in spirit to the zero temperature limit of the Glauber dynamics, but is still slightly different. In the Glauber case, all transitions that lower the energy would be treated as equivalent, and one among them would be chosen randomly, whereas the procedure used here is purely deterministic.

The basic interpretation of glassy dynamics in phase space is that IS with lower and lower energies are visited during the aging regime, or at equilibrium when decreasing temperature. In a loose sense, IS with lower and lower energies may be considered as ‘closer’ to the ground state. So from a real space point of view, one might expect these ‘deep’ IS to minimize the energy at least over some small parts of the system. To give a well defined meaning to these intuitive ideas, we propose the following procedure. Picking up two sites \( i \) and \( j = i + \xi \), we search for the configuration \( \{ \tilde{q}_k \} \) which minimizes the energy upon the interval \([i, j]\), with the fixed boundary conditions \( \tilde{q}_i = q^\text{IS}_i \) and \( \tilde{q}_j = q^\text{IS}_j \). Then the configuration \( \{ \tilde{q}_k \} \) is compared with \( \{ q^\text{IS}_k \} \) over the interval \([i, j]\). If both configurations coincide, a larger value \( \xi' = \xi + 1 \) (\( \xi = 2 \) in the initial step) can then be tested, changing \( j \) and keeping \( i \) fixed. The procedure is iterated until the largest interval over which \( \{ \tilde{q}_k \} \) and \( \{ q^\text{IS}_k \} \) coincide is found; the corresponding value of \( \xi \) is denoted as \( \xi_i \). Repeating the procedure for all sites \( i \), a set of domains \( D_i = [i, i + \xi_i] \) (\( i = 1, \ldots, N \)) is obtained. Yet, some of these domains are actually included in a larger one, since it may happen that \( i + \xi_i = (i + 1) + \xi_{i+1} \); in this case, \( D_{i+1} \) is included in \( D_i \). Keeping only the intervals \( D_i \) that are not included in a larger one, one finds a non trivial decomposition into almost non overlapping space intervals, over which the IS considered minimizes the energy.

The distribution \( P(\xi, t) \) of the size of these regions has been computed numerically for different times \( t \)—see Fig. 2(a)—and is seen to be exponential, at least for \( \xi \gtrsim 4 \). From this distribution, the characteristic size \( \xi^*(t, T) \) at time \( t \) and temperature \( T \) can be deduced from the slope of the exponential; \( \xi^*(t, T) \) is plotted on Fig. 2(b) for different temperatures. These simulations were done with relatively small systems (\( N = 100 \)), since the computation time grows like \( N^2 \), and results were averaged over a large number of realizations (from \( 10^3 \) to \( 2 \times 10^4 \)). We have checked over larger systems that finite size effects are small.

As expected intuitively, the characteristic length scale \( \xi^*(t, T) \) increases during the aging regime before saturating to its equilibrium value at large times. One can see that the shape of the curves depends only weakly on temperature, once correctly rescaled—see inset of Fig. 2(b). The fact that data rescale as a function of \( T \ln t \) indicates that activation effects play an im-

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**Fig. 3** — (a) \( \xi^*(t, T) \) for different values of \( M \) (\( T = 0.5 \)). (b) Equilibrium length \( \xi_{eq}(T) \) for \( M = 10 \).

Inset: same data as a function of \( 1/T \), and linear fit \( \xi_{eq}(T) \approx a/T - b \) (\( a = 7.31 \), \( b = 2.21 \)).
important rôle in the model. The length $\xi^*(t, T)$ also displays important quantitative variations with the value of $M$, as seen from Fig. 3(a). Yet, the qualitative behavior remains the same for all $M$. On the other hand, the equilibrium length $\xi_{eq}(T)$, obtained from the long time limit of $\xi^*(t, T)$, increases markedly (as $1/T^2$) when temperature is lowered –see Fig. 3(b).

One can wonder whether some of the domains found above coincide with the global ground state of the system. Interestingly, numerical tests show that this is indeed the case, and that domains coinciding with the latter alternate with domains which do not coincide. Let us denote by $\xi^*_e$ the typical size of these ‘excited domains’, i.e. domains that differ from the ground state. This typical size $\xi^*_e$ need not be the same as the overall characteristic length $\xi^*$, since domains coinciding with the ground state may be significantly larger than the excited ones. Indeed, numerical simulations show that $\xi^*_e$ decreases during the aging regime at fixed temperature, as seen on the inset of Fig. 4(a), and becomes much smaller than $\xi^*(t, T)$ –see Fig. 2(b) for comparison. So we come up with the following picture for the present model: at large time after a quench, or in the equilibrium regime, an IS may be thought of as a set of small excited domains on top of the ground state. Moreover, the typical size of these excitations becomes rather small in comparison with the global average size.

To proceed further, it would be necessary to know the energy distribution of the excited domains. In order to sample the IS in a uniform way, we quench the system directly from infinite temperature to determine the IS, and record the energies (defined with respect to the ground state) of the excited domains. The corresponding distribution $P(E)$ is shown in Fig. 4(a), and is found to be exponential, except for small energies. We can now test whether this picture is able to make some relevant predictions concerning the equilibrium length $\xi_{eq}(T)$, and in particular its $1/T$ behavior. For simplicity, we assume that the distribution $P(E)$ is purely exponential (discarding the deviations at small $E$): $P(E) = \lambda \exp(-\lambda E)$, with $\lambda = 0.159$ from the numerical data. In equilibrium at temperature $T$, the concentration $c(E)$ of excited domains with energy $E$ can be estimated as $c(E) = 1/[1 + \exp(E/T)]$ (see e.g. [18]). The global concentration $\bar{c}$ of excited domains is then computed as the average of $c(E)$ over the distribution $P(E)$:

$$\bar{c} = \int_0^\infty dE P(E) c(E) = \int_0^\infty dE \frac{\lambda e^{-\lambda E}}{1 + e^{E/T}}$$  \hspace{1cm} (2)
Evaluating the last integral for $T \to 0$ yields $\tau \approx \lambda T \ln 2$. The typical distance between these (small size) excited domains is given by $\xi = 1/\tau = \tilde{a}/T$, with $\tilde{a} = 1/(\lambda \ln 2)$. This distance is precisely the size of the large domains (i.e. those that coincide with the ground state), which actually dominate the distribution $P(\xi, t)$ of domain sizes. Thus this simple argument is indeed able to predict the correct $1/T$ behavior of $\xi_{eq}(T)$ at low temperature. The predicted slope $\tilde{a} = 9.07$ is in rather good agreement with the slope $a = 7.31$ found from Fig. 3(b) given the crude approximations made in the above argument.

**Discussion.** – A similar decomposition of the IS into domains of minimum energy already appears in the study of the disordered Ising chain [17], but with emphasis on the computation of configurational entropy rather than on the notion of characteristic length scale. Indeed, in the disordered Ising chain, the introduction of the notion of ‘weak links’ [17] (i.e. links that may be either frustrated or not, in an IS) leads straightforwardly to the identification of domains upon which the energy is minimized, in a way quite similar to what happens in the present model. Yet, to get closer to the present situation, one should rather consider the disordered Ising chain in the presence of a small external field, in order to avoid the degeneracy of the ground state. One then expects to find some excitations on top of the ground state, just as in the present model.

An open question is to know whether the length scale $\xi^*(t, T)$ characterizing the IS is the same as the length scale $\xi_{4p}$ found from the usual (two-replica) four-point correlation function. In other words, are the instantaneous configurations characterized by the same length scale as the IS? To check this point, we have computed the four-point correlation function $C_{ab}(r, t)$ associated to two copies $a$ and $b$ of the system, with the same disorder, and defined as:

$$C_{ab}(r, t) = \frac{\langle S_i(t)S_{i+r}(t) \rangle - \langle S_i(t) \rangle^2}{\langle S_i(t)^2 \rangle - \langle S_i(t) \rangle^2} \quad (3)$$

where $S_i(t)$ is a short notation for $\delta_{q^a(t)q^b(t)}$. The length scale $\xi_{4p}$ characterizing the decay of $C_{ab}(r, t)$ is plotted on Fig. 4(b) as a function of time, for $T = 0.5$. One sees that it remains quite small, of the order of one or two lattice spacings.

Still, the situation is actually complicated by the fact that the quantities used to measure the length scales are different (correlation function versus distribution of domain sizes), which induces some systematic bias. Indeed, one can apply the procedure of local energy minimization defined earlier in this paper for the IS, to the instantaneous configurations visited dynamically by the system, without looking to the associated IS. Interestingly, the distribution of domains found in this way still has an exponential shape; the corresponding characteristic length scale $\xi_{dyn}$ is plotted on Fig. 4(b). Interestingly, $\xi_{dyn}$ appears to be much closer to $\xi^*$ than $\xi_{4p}$. When lowering the temperature, $\xi_{dyn}$ and $\xi^*$ become even closer – data not shown. This may not be surprising if one considers that IS are obtained from instantaneous configurations by (partially) removing the thermal noise. As a result, it seems that IS and instantaneous configurations are essentially characterized, at least in the present model, by the same length scales – although they look quite different when comparing $\xi^*$ and $\xi_{4p}$.

Nevertheless, one may expect these two length scales to differ in some models, as can be seen from the (non-disordered) zero field Ising model. In this model, the IS are either the two ground states, or more complicated structures [19], but they are in any case characterized by a length scale of the order of the system size. On the contrary, the dynamical configurations are characterized by a finite correlation length in equilibrium, and a finite (although growing

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(1)If the IS are determined by a quench with a zero temperature Glauber dynamics, then non trivial IS appear in the Ising model in dimension two and above; in two dimensions, these IS are made of alternating stripes of up and down spins [19].
with time) typical domain size in the coarsening regime. Thus these two length scales are indeed different in the Ising model—which is a limiting case where one is infinite in the thermodynamic limit. So it would be very interesting to see if there exists some models for which both lengths would be finite, while evolving in independent ways.

Conclusions. – To conclude, we have introduced an analysis of IS in terms of domains upon which energy is minimized. The size of these domains is distributed exponentially, and the average size grows with time at fixed temperature. The equilibrium length, reached at large times, increases as $1/T$ when lowering temperature $T$, which can be interpreted within a simple picture of excited domains. Besides, this method gives more information than simply comparing the IS with the ground state, since it shows that domains that do not coincide with the fundamental still minimize locally the energy.

These results call for future work in order to extend the present procedure to higher space dimensions. Although this extension may not be trivial, it should be an important step toward the understanding of the real space properties of IS. In addition, it would be very interesting to investigate in different models the relation between the length scale characterizing the IS and the one resulting from the two-replica correlation function. Either these two length scales should be different at least in some specific models, or the reason for their identity should be understood.

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