Facilitated spin models on Bethe lattice: bootstrap percolation, mode-coupling transition and glassy dynamics

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Abstract. – We show that facilitated spin models of cooperative dynamics introduced by Fredrickson and Andersen display on Bethe lattices a glassy behaviour similar to the one predicted by the mode-coupling theory of supercooled liquids and the dynamical theory of mean-field disordered systems. At low temperature such cooperative models show a two-step relaxation and their equilibration time diverges at a finite temperature according to a power-law. The geometric nature of the dynamical arrest corresponds to a bootstrap percolation process which leads to a phase space organization similar to the one of mean-field disordered systems. The relaxation dynamics after a subcritical quench exhibits aging and converges asymptotically to the threshold states that appear at the bootstrap percolation transition.

Introduction. – Lattice models are widely used in statistical mechanics to gain a qualitative and often deeper understanding of physical phenomena. In a seminal work Fredrickson and Andersen (FA) [1] introduced a simple lattice spin model of the liquid-glass transition, whose Hamiltonian corresponds to uncoupled Ising spins in a positive magnetic field [2, 3]. The spins represent a coarse-grained region of the liquid with high (-1 spins) or low ($+1$ spins) mobility and the magnetic field, that favors up spins, leads to very few mobile regions embedded in an immobile background at low temperature. The spin dynamics is subjected to a *kinetic constraint*: for each time step a randomly selected spin can flip only if the number of nearest neighbor down spins is larger or equal than f, where the facilitation parameter f is a number between zero and the lattice connectivity. The kinetic constraint mimics at a coarse grained level the cage effect in super-cooled liquids, where particles rattle in the cage formed by their neighbors and then move further if they are able to find a way through the surrounding particles. At low temperature/high density the latter process is strongly inhibited leading to an arrest of particle motion over macroscopic time scales. Similarly, at high temperature the kinetic constraint plays a little role and the relaxation is fast, whereas at low temperature

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(i.e. high density of up spins) it is hardly satisfied and relaxation involves strongly cooperative processes which can be exceedingly slow. The basic assumption behind this approach is that the slow dynamics in glass-forming liquids is *not* due to a thermodynamic transition (there is no singularity in the partition function of non-interacting Ising spins in a magnetic field), but rather to a purely dynamic mechanism.

Kinetically constrained models (KCM), such as the FA and the KA model [4], encode in a very compact way many features of real glass-forming systems. Stretched exponential relaxation [2], super-Arrhenius equilibration time [3], dynamical heterogeneity [5] and self-diffusion/viscosity decoupling [6] are some examples. They also display basic glassy features, such as physical aging [7] and effective temperature [8], first derived in the out of equilibrium dynamics of random p-spins systems [9]. In finite dimensions no transition takes place at finite temperature (or non-unit density) [10,11], while on Bethe lattices a dynamical transition similar to that predicted by the mode coupling theory (MCT) may occur [11–13].

The nature of this similarity is far from being obvious. On one hand, KCM are defined by *ad hoc* kinetic rules which, although physically motivated, have little to do with the microscopic (Newtonian or Brownian) dynamics of glass-forming liquids. On the other hand, most results concerning the aging dynamics were derived within fully connected spin-glasses, which unlike KCM have built-in quenched disorder and a non-trivial thermodynamics at low temperature (characterised by a replica-symmetry broken phase). In order to make further progress in this direction we investigate the relaxation dynamics of the FA model on a Bethe lattice. (In a recent work motivated by similar issues [14], MCT has been applied to 1D FA model). We show in detail that the mechanism of ergodicity breaking can be understood in terms of *bootstrap percolation* (as already mentioned in Refs. [10–13]), and that the phase space organization and several dynamical features are well described by the predictions of MCT and its out of equilibrium generalisation [9].

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FA model on Bethe lattice and the bootstrap percolation. – The FA model we consider in this paper consists of N Ising spin variables, $\sigma_i = \pm 1$, $i = 1, \dots, N$, on a Bethe lattice with connectivity k. The denomination Bethe lattice refers here to a random regular k-graph, that is a graph taken at random within the set of graphs with fixed connectivity $z = k+1$ on each site. In this random graph all sites are on the same footing, and there is no "surface" effect. The Hamiltonian is simply: $H = -\frac{1}{2}\sum_i \sigma_i$, and the spin dynamics is subjected to a kinetic constraint: at each time step a randomly chosen spin is flipped with the rate: $w(\sigma_i \to -\sigma_i) = \min\left\{1, \mathrm{e}^{-\beta\sigma_i}\right\}$, *only if* the number of nearest neighbor in state -1 is larger than or equal to f ($\beta = 1/T$ is the inverse temperature). FA models with $f > 1$ are usually called cooperative since their relaxation time grows faster than the Arrhenius law at low temperature, at variance with the simpler non-cooperative case $f = 1$. In the literature it seems to be known, even if not discussed in detail, that the FA model on a Bethe lattice has an ergodic/non-ergodic transition at a finite temperature for $k > f > 1$ [12,13]. This is closely related to the bootstrap percolation transition, as we will explain in the following.

The local structure of a Bethe lattice is Cayley-tree like with k branches going up from each node and one going down. Let us call B the probability that, without taking advantage of the configuration on the bottom, the spin σ_i is in the state -1 or can be brought in this state rearranging the sites above it. B verifies a simple iterative equation:

$$B \;=\; (1-p) + p\sum_{i=0}^{k-f}\binom{k}{i}B^{k-i}(1-B)^i \tag{1}$$

where $p = 1/(1+\mathrm{e}^{-1/T})$ is the probability that the spin is $+1$ in thermal equilibrium. Eq. (1)

has, for small p (i.e. high-temperature) only the solution $B = 1$: with probability one each spin can be flipped in the up-state using a certain (finite) number of allowed moves. At low temperature, when p is large enough, a transition occurs to a fixed point $B < 1$ for any choice of $k > f > 1$ (the critical value of p depending on k and f). The properties of this blocking (or jamming) transition can be easily established. For arbitrary small $1 - B$ the eq. (1) becomes $(1 - B) = p\binom{k}{f-1}(1 - B)^{k-f+1} + \ldots$ Since the power of $1 - B$ on the right and left hand side are different only a discontinuous transition is possible for $k > f$. One can also show that if $1 - p$ (i.e. the temperature) is small enough then a transition has to take place. Furthermore at the transition it is easy to check that $1-B$ has a square root singularity coming from low temperatures. This mixed character of first and second order is similar to the behavior of the non-ergodicity parameter in MCT. Notice also that there is no transition for the non-cooperative case $f = 1$ (no matter the value of k). Let us now explain how the above transition is related to the bootstrap percolation (BP), [15, 16]. In BP each site of a lattice is first occupied by a particle at random with probability p. Then, one randomly remove particles which have less than $m = k - f + 2$ neighbors. Iterating this procedure leads to two possible asymptotic results [16]. If the initial particle density is larger than a given threshold p_c there is a residual infinite cluster of particles that remains at the end of this procedure, whereas for $p < p_c$ the density of residual particles is zero. In ref. [16] it has been shown that the probability P that a particle is blocked because it has more than $k - f + 1$ neighboring particles above it which are blocked (without taking advantage of vacancies below) satisfies the eq. $P = p\sum_{i=0}^{f-1}\binom{k}{i}P^{k-i}(1 - P)^i$. Changing variable $i' = k - i$ and the notation particle-vacancy/up-down spin one obtains that $1 - P$ verifies the same equation of B. Thus the two transitions coincide. In fact, if $P > 0$ then there will be particles (spins) blocked permanently and $B < 1$. If $P = 0$ then there exists, with probability one, a sequence of allowed moves that brings a random equilibrium configuration to the configuration with all sites -1 by definition (this set of configurations has been called the high temperature partition by Fredrickson and Andersen). Hence, each site can flip to -1 after a certain number of allowed moves and $B = 1$. Although irreducibility is not equivalent to ergodicity we expect that, because of the trivial thermodynamic measure, the bootstrap and dynamical transition coincide. Of special interest is the fraction ϕ of spins that are permanently frozen. It can be computed exactly from P as:

$$\phi \;=\; p\sum_{i=0}^{f-1}\binom{k+1}{i}P^{k+1-i}(1-P)^i + (1-p)\sum_{i=0}^{f-1}\binom{k+1}{i}(ph_{k,f})^{k+1-i}(1-ph_{k,f})^i\,, \quad (2)$$

where $h_{k,f} = \sum_{i=0}^{f-2}\binom{k}{i}P^{k-i}(1 - P)^i$. The two contributions are respectively the probability that a spin is frozen in the state ± 1. In the following we analyze the case $f = 2$, $k = 3$, which mimics the square lattice with $f = 2$. In this case $P = p\left(P^3 + 3P^2(1 - P)\right)$, and the critical value of p at which the transition takes place is $p_c = \frac{8}{9}$ which gives $T_c = 1/\ln\frac{p_c}{1-p_c} = 0.480898$. The corresponding fraction of frozen spins is $\phi_c = \phi(T_c) \simeq 0.67309$.

Equilibrium dynamics and relaxation time. – The equilibrium dynamics of KCM is usually analyzed in terms of the persistence function $\phi(t)$, i.e. the probability that a spin has never flipped between times 0 and t [17]. The analytical results obtained above for the fraction of frozen spins are directly relevant to the long-time limit of $\phi(t)$ that indicates when the ergodicity is broken:

$$\lim_{t\to\infty}\phi(t) = 0\,,\ \text{for}\ \ T > T_c\,; \qquad \lim_{t\to\infty}\phi(t) > 0\,,\ \text{for}\ \ T \le T_c \quad (3)$$

and therefore it plays the same role of the non-ergodicity parameter in supercooled liquids, and the Edwards-Anderson parameter in spin-glasses. In order to compare the above results

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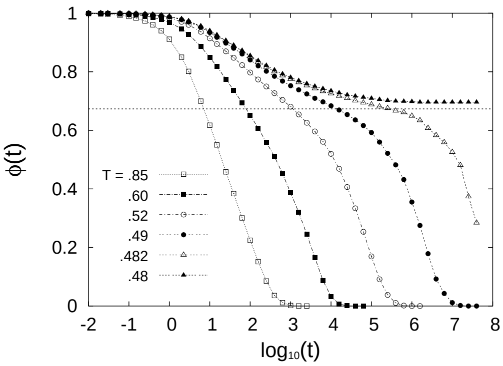

Fig. 1

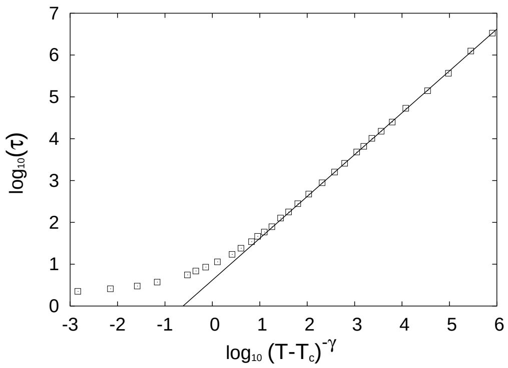

Fig. 2

Fig. 1 – Persistence function $\phi(t)$ vs time t during the equilibrium dynamics at temperatures T, for a FA model with facilitation parameter $f = 2$, on a Bethe lattice with connectivity $k + 1 = 4$. The straight line is the plateau ϕ_c predicted by the bootstrap percolation argument. System size $N = 2^{18}$.

Fig. 2 – Integral relaxation time τ vs temperature T. The dynamical critical temperature T_c is the one predicted by the bootstrap percolation argument, $T_c \simeq 0.481$. The power-law exponent is $\gamma \simeq 2.9$.

with numerical simulation we have implemented a faster than the clock Monte Carlo code [18] for the dynamics of the FA model on a Bethe lattice. In fig. 1 we show the persistence function $\phi(t)$ for $f = 2$, and $k = 3$. The data are obtained by using an initial configuration with equilibrium magnetization $m = \tanh(\beta/2)$ which is by construction a typical equilibrium configuration. Upon decreasing T towards T_c, $\phi(t)$ develops a clear two-step behavior in which the density of frozen spins slowly approaches a plateau, and then decay to zero on longer time scale. Similar results are obtained for the spin-spin correlation function. The plateau value is equal to the fraction of spins that never flip, see eq. (2). The estimated values of T_c and ϕ_c are in good agreement with the theory. We have also obtained the relaxation time, $\tau(T)$, as the integral of the persistence function. Consistently with the prediction $\tau(T)$ diverges at a finite temperature exactly given by $T_c \simeq 0.48$. Moreover, we find that the divergence has a power-law singularity $\tau(T) \sim (T - T_c)^{-\gamma}$, with an exponent $\gamma \simeq 2.9$, see fig. 2. This behavior is observed over five decades of relaxation time and holds for any temperature below 1. We also mention that at low temperature, the departure from the plateau is well described by the von Schweidler law, while the late stage of relaxation (the so-called α regime) obeys the time-temperature superposition principle, $\phi(t) = \Phi(t/\tau(T))$, the scaling function Φ being fitted well by a Kohlrausch-Williams-Watts stretched exponential. Since the BP has features of both first and second order transitions we expect increasing fluctuations on approaching T_c. Such fluctuations have a purely dynamical nature as being related to the dynamical order parameter $\phi(t)$ and can be detected by measuring the dynamical susceptibility $\chi(t) = N(\langle\phi^2\rangle - \langle\phi\rangle^2)/T$. We observe indeed that $\chi(t)$ develops a peak (see fig. 3) that diverges as $\tau(T)$ for $T \to T_c$, similarly to what has been found in random p-spin model and MCT [19, 20].

Energy relaxation and the threshold states. – To better understand the glassy behaviour of the FA model on Bethe lattice we have studied the aging dynamics and the phase-space organization below T_c. For comparison, it is useful to recall the scenario of mean-field disordered models of structural glasses [9, 21]. Below a temperature T_d ergodicity is broken, and the configuration space decomposes in an exponential number (in the system size) of ergodic

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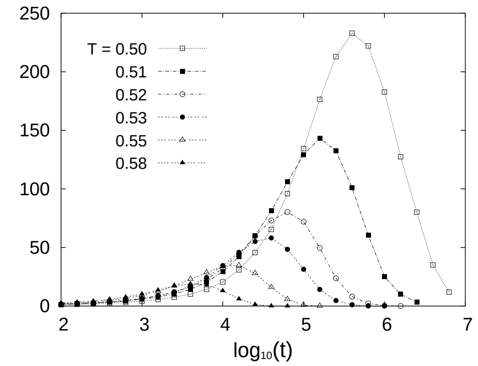

Fig. 3

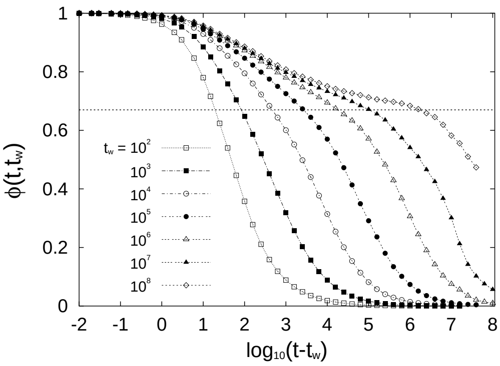

Fig. 4

Fig. 3 – Equilibrium dynamical susceptibility $\chi(t)$ vs time t at temperature T. System size $N = 2^{14}$.

Fig. 4 – Two-time persistence $\phi(t, t_{\rm w})$ after a subcritical quench at temperature $T = 0.4$. The straigth line is the (temperature-independent) plateau $\phi_{\rm c}$ predicted by the bootstrap percolation argument.

components or TAP states (corresponding to different minima of the local magnetization free energy functional, i.e. the TAP free energy). The logarithm of the number of states, the configurational entropy, jumps from zero to a finite value at $T_{\rm d}$. The TAP states which dominate the Boltzmann weight at $T_{\rm d}$ are called *threshold states* and play an important role in the dynamical behaviour. Relaxational dynamics at $T < T_{\rm d}$, starting from a random configuration exhibits aging: the system approaches asymptotically the threshold states being unable to thermalise within any TAP state at temperature T. One time observables, like the energy, converge asymptotically to the corresponding threshold value, while two-time correlation and response functions do not obey the usual equilibrium fluctuation-dissipation relation. This scenario has relevance beyond the physics of glassy systems: a striking example is the typical-case analysis of hard combinatorial optimization problems [22]. Note however that disordered systems may have an aging dynamics dominated by different layers of TAP states depending on the cooling schedule [23]. In the following we check if the scenario outlined above is relevant to the FA model. The counterpart of a TAP state in the FA model will be the set of all configurations having the same backbone of frozen spins.

We generally find that after a subcritical quench at temperature T the energy approaches an asymptotic value, $e_\infty(T)$, above the equilibrium one, $e_{\rm eq}(T) = -\tanh(1/2T)/2$. Accordingly, the two-time persistence between time $t_{\rm w}$ and t shows a two-step aging behavior, see fig. 4. In fig. 5 we plot the excess energy $\Delta e(t) = (e_\infty(T) - e(t))/(e_\infty - e(0))$ for $T = 0.47$. After a short-time temperature-independent exponential relaxation, $\Delta e(t)$ decays according to a power-law $\Delta e(t) \sim t^{-\nu}$. A similar behavior is observed for different quenching temperatures, with ν varying in the range [0.31, 0.34] for $T \in [0.34, 0.48]$. In fig. 6 we compare $e_\infty(T)$, with the energy density of the threshold states $e_{\rm th}(T)$. The latter is obtained by cooling (heating) at a slow enough rate $\dot\epsilon$ a random equilibrium configuration at $T_{\rm c}$. In this way the system reaches equilibrium within one of the ergodic components and its energy at temperature T represents, in the limit $\dot\epsilon \to 0$, the threshold energy. We find that for T not too far from $T_{\rm c}$ the results obtained with the two protocols are equal within the numerical accuracy, see fig. 6. For $T \ll T_{\rm c}$, we cannot exclude a small discrepancy between $e_{\rm th}(T)$ and $e_\infty(T)$ due to the difficulty to access the asymptotic dynamics in the available time window. This equality is by no means trivial and strongly suggests that the threshold states dominate indeed the

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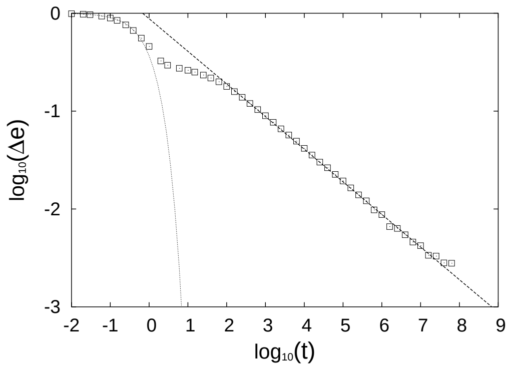

Fig. 5

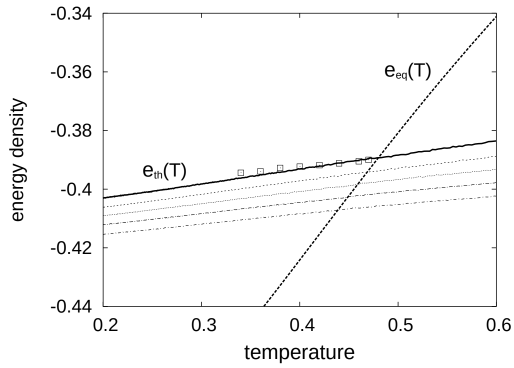

Fig. 6

Fig. 5 – Excess energy density $\Delta e(t) = (e_\infty(T) - e(t))/(e_\infty(T) - e(0))$ vs time t, after a subcritical quench at temperature $T = 0.38$. The dashed line is a power-law $\Delta e(t) \sim t^{-\nu}$ with $\nu \simeq 0.33$. The dotted line is a temperature-independent exponential relaxation.

Fig. 6 – The dashed line is the equilibrium energy $e_{\rm eq}(T) = -\tanh(1/2T)/2$. The full line is the threshold energy $e_{\rm th}(T)$ obtained by cooling (heating) a configuration equilibrated at $T_{\rm c} \simeq 0.48$. Square symbol represents the asymptotic energy, $e_\infty(T)$, of a subcritical quench at temperature T. Four subthreshold states are also shown; they are obtained by cooling (heating) an equilibrium configuration at temperature $T = 0.47$, 0.46, 0.45, and 0.44.

off-equilibrium behavior. Subthreshold states with $e_{\rm TAP}(T) < e_{\rm th}(T)$ are sampled by considering an initial equilibrium configuration at $T < T_{\rm c}$. These states represent different ergodic components and are completely separated from each other in the dynamical evolution. They can be followed by varying the temperature and their phase space organization is very similar to the one of p-spins models (for comparison see fig. 1 in ref. [21]). The main difference is that TAP states in the FA model are stable against thermal fluctuations: upon heating they never disappear (i.e. $T_{\rm TAP} = \infty$ in the notation of ref. [21]) This is a consequence of the athermal nature of the blocking transition, which in our case is due to a purely kinetic, rather than geometric, constraint. We find blocked structures even above $T_{\rm c}$ but they have a vanishing Boltzmann weight and are not seen by the off-equilibrium dynamics.

Conclusion. – We have studied facilitated spin models of glassy dynamics on a Bethe lattice with fixed connectivity $k+1$ and facilitation parameter f. For the non-cooperative case, $f = 1$, there is no transition at non-zero temperature, the relaxation time is Arrhenius, and no two-step relaxation is observed. The cooperative case, $k > f > 1$, is much richer: at a finite temperature $T_{\rm c}$ a giant cluster of frozen spins appears and hence ergodicity is broken. The transition presents a mixed character: the fraction of frozen spins jumps discontinuously at $T_{\rm c}$ with a square root singularity, and therefore there are critical fluctuations with diverging correlation length and time scales. The relaxation time diverges as a power-law at $T_{\rm c}$, and a two-step relaxation is observed both in and out of equilibrium. The geometric mechanism behind such a jamming transition is a bootstrap percolation phenomenon, as pointed out previously [11–13]. The onset of jamming in sphere packings and its relation with the bootstrap or k-core percolation [25], and rigidity percolation [26] has been recently discussed in ref. [24]. Microscopically this transition is rather different from the dynamic transition occurring in mean field disordered systems [27]. In spite of this, we have shown that several characteristics of the glassy dynamics studied above are remarkably similar to those found in

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the mode-coupling theory and the aging dynamics of mean-field models of structural glasses. This seems to be related to the emergence of a very similar organization of the phase space, in which the sets of configurations having the same backbone of frozen spins play the role of TAP states. In finite dimension the Bethe lattice glass transition is replaced by a possibly sharp crossover, as recently shown for the KA model [11]. Finite-size systems also exhibit a blocking transition at a finite temperature, due to the exceedingly slow approach to the thermodynamic limit in bootstrap percolation problems [15, 28]. Numerical evidences suggest that some peculiar features of mean-field structural glasses remain even in finite dimension, at least on long but finite time-scales [8, 29]. Further work would be certainly valuable to improve the understanding of this crossover.

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