Glass transition in models with controlled frustration

Annalisa Fierro
INFM-Coherentia, Dipartimento di Scienze Fisiche, Università di Napoli "Federico II," Complesso Universitario Monte Sant'Angelo, Via Cinthia, I-80126, Napoli, Italy

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A class of models with self-generated disorder and controlled frustration is studied. Between the trivial case, where frustration is not present at all, and the limit case, where frustration is present over every length scale, a region with local frustration is found where glassy dynamics appears. We suggest that in this region, the mean field model might undergo a p-spin like transition, and increasing the range of frustration, a crossover from a 1-step replica symmetry breaking to a continuous one might be observed.

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The study of spin glasses and glassformers has shown that these systems present similar complex dynamical behaviors. In particular the dynamical equations of p-spin models [1], a generalization of the spin glass model in mean field, coincide above the dynamical transition temperature with the mode coupling equations for supercooled liquids [2]. However the connection in finite dimension between spin glasses and glassformers is not completely clear. On the one hand, spin glasses undergo a thermodynamic transition at a well defined temperature, where the nonlinear susceptibility diverges. The systems that show a transition of this kind, in spite of very different microscopic structures, have two essential common characteristics: The presence of competitive interactions (frustration) and quenched disorder. On the other hand, glassformers are a class of systems where disorder is not originated by some fixed external variables, but is "self-generated" by the particle positions and orientations. Moreover there is no sharp thermodynamic transition characterized by the divergence of a thermodynamic quantity analogous to the nonlinear susceptibility. In order to clarify the connection and the differences between glasses and spin glasses, and to investigate the roles of disorder and frustration in the behaviors observed, in the present paper we study a class of models with annealed interactions and controlled frustration.

We consider a diluted spin glass, the frustrated lattice gas (FLG) [3], constituted by diffusing particles, and therefore suited to study quantities like the diffusion coefficient, or the density autocorrelation functions, important in the study of liquids. The Hamiltonian of the model is:

$$-\mathcal{H} = J\sum_{\langle ij\rangle} (\epsilon_{ij}S_iS_j - 1)n_in_j + \mu\sum_i n_i, \tag{1}$$

where $S_i=\pm 1$ are Ising spins, $n_i=0,1$ are occupation variables, and $\epsilon_{ij}=\pm 1$ are ferromagnetic and antiferromagnetic interactions between nearest neighbor spins. This model was studied both for quenched [3,4] and annealed interactions [5]: In the quenched case the interactions, ϵ_{ij}, are quenched variables randomly distributed with equal probability; in the annealed case ϵ_{ij} evolve in time.

In the limit μ/T goes to infinity all sites are occupied ($n_i\equiv 1$ for each site i), and the quenched model reproduces the Ising spin glass. In the other limit, $T/J=0$, the model, Eq. (1), has properties recalling a "frustrated" liquid. Indeed the first term of the Hamiltonian implies that two nearest neighbor sites can be freely occupied only if their spin variables satisfy the interaction, that is if $\epsilon_{ij}S_iS_j=1$, otherwise they feel a strong repulsion. Since in a frustrated loop the spins cannot satisfy all the interactions, in this model particle configurations in which a frustrated loop is fully occupied are not allowed. The frustrated loops in the model are the same of the spin glass model and correspond in the liquid to those loops which, due to geometrical hindrance, cannot be fully occupied by the particles.

Here we study a class of annealed FLG models defined by the following partition function:

$$\mathcal{Z}_{an} = \sum_{\{\epsilon\}}^{*}\sum_{\{\sigma\}} e^{-\beta\mathcal{H}}, \tag{2}$$

where $\mathcal{H}$ is given by Eq. (1), the sum $\Sigma_{\{\sigma\}}$ is over all the possible configurations of spin and particles $\{\sigma\}\equiv\{S_i,n_i\}$, and the sum $\Sigma^*_{\{\epsilon\}}$ is over all the possible interaction configurations such that the annealed averages of the frustrated loop number coincide with the quenched ones for every length of the loops until a maximum value, $r_{\max}$ ($r_{\max}=0,4,6,8,\cdots$ on a cubic lattice). Varying $r_{\max}$ from zero to infinity a class of models with controlled frustration is obtained. In the limit, $r_{\max}=0$, frustration is not present at all: the model [5] is equivalent to a lattice gas with a repulsion between nearest neighbors, and without frustration and correlations between spin, and no thermodynamic transition is present. In the other limit, $r_{\max}$ goes to infinity, frustration is present over every length scale, as in the quenched case: We expect that the partition function, Eq. (2), coincides with the quenched one, namely the model undergoes a spin glasslike transition [4], as shown in Ref. [6] for the Ising spin glass model [7]. For intermediate values of $r_{\max}$ a class of models with local frustration and self-generated disorder is obtained.

In the present paper the models, Eq. (2), have been studied for $r_{\max}=4$ and $r_{\max}=6$: In the first case a trivial dynamical behavior is observed, with one step relaxation functions and a smooth increasing of relaxation time as function of density; in the second case a dynamical behavior very similar to that of glass formers is instead found. We therefore observe that by increasing the degree of frustration the system

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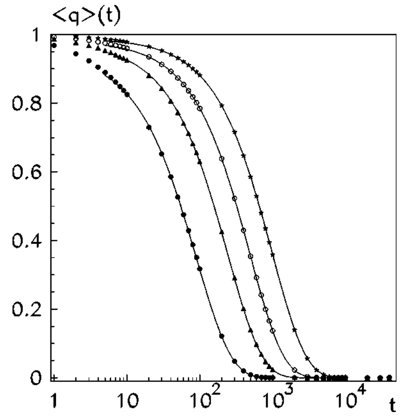

FIG. 1. The relaxation functions of the self-overlap, $\langle q\rangle(t)$, for $r_{\max}=4$ at the densities $\rho=0.63$, 0.70, 0.74, 0.76 (from left to right). The continuous curves in figure are stretched exponential functions with $\delta=0.93$.

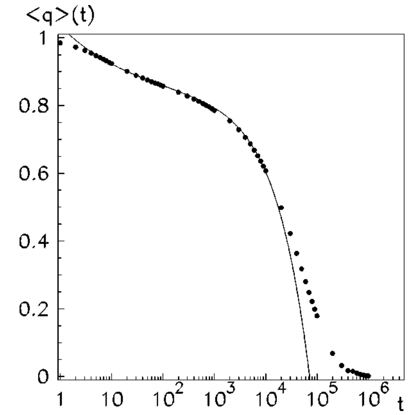

FIG. 3. The relaxation functions of the self-overlap, $\langle q\rangle(t)$, for $r_{\max}=6$ at the density $\rho=0.69$. The curve in figure is the β-correlator of the MCT with exponent parameters $a=0.327$ and $b=0.641$, and plateau height $f_0=0.84$.

moves from a liquidlike to a glassylike behavior.

The system was simulated using Monte Carlo techniques over a cubic lattice of linear size $L=8$. At the beginning the interactions, $\epsilon_{ij}=\pm 1$, are randomly distributed with equal probability. At each step of the dynamics an attempt to move a particle to a nearest neighbor site (the spin is flipped with a probability equal to $1/2$) is alternated with an attempt to exchange two nearest neighbor interactions: in the limit here considered, $T/J=0$, a particle can move to a nearest neighbor site only if its spin satisfies the interactions with all the new nearest neighbors, and an interaction can be changed only if at least one of its extreme is empty. The frustrated loop numbers of any fixed length until $r_{\max}$ are independently kept constant during the dynamics.

At a given value of the density, ρ, we calculated the two-time relaxation function of the self-overlap, $C(t,t_w) = 1/N_p\sum_{i=1}^{L^3}\overline{S_i(t_w)n_i(t_w)S_i(t)n_i(t)}$, where N_p is the number of particles, and the average $\overline{\cdots}$ is done over 8–32 different realizations of the system. For values of t_w long enough, the system reaches a stationary state, where the time translation invariance is recovered, i.e., $C(t,t_w)=C(t-t_w)$. In this time region we calculated the equilibrium relaxation function of the self-overlap:

$$\langle q\rangle(t) = \frac{1}{N_p}\sum_{i=1}^{L^3}\langle S_i(t)n_i(t)S_i(t+t')n_i(t+t')\rangle, \tag{3}$$

and the dynamical nonlinear susceptibility [9]:

$$\chi(t) = N_p(\langle q^2\rangle(t) - \langle q\rangle^2(t)). \tag{4}$$

Here $\langle\cdots\rangle$ is the time average on time t'. For each density the quantities of interest are averaged over $8-32$ different realizations of the system, and the errors are calculated as the fluctuations over this statistical ensemble.

We first consider the model with $r_{\max}=4$: Since $r_{\max}$ equals the loop minimum length, the interactions evolve under the constraint that the number of frustrated loops of length 4 is kept constant. In this case, both $\langle q\rangle(t)$ and $\chi(t)$ show a liquidlike behavior also at high densities: $\langle q\rangle(t)$, plotted in Fig. 1, relaxes with a one step decay well fitted by a stretched exponential function, $f(t)=A\exp\{-(t/\tau)^{\delta}\}$, with δ

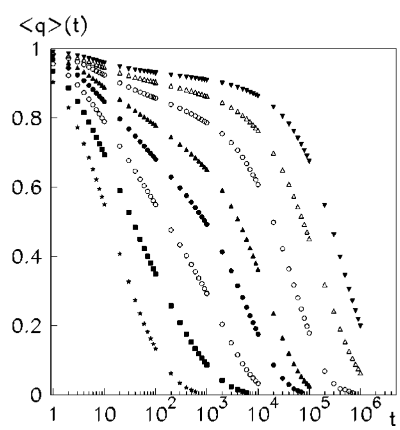

FIG. 2. The relaxation functions of the self-overlap, $\langle q\rangle(t)$, for $r_{\max}=6$ at the densities $\rho=0.48$, 0.54, 0.59, 0.63, 0.66, 0.71, 0.73 (from left to right).

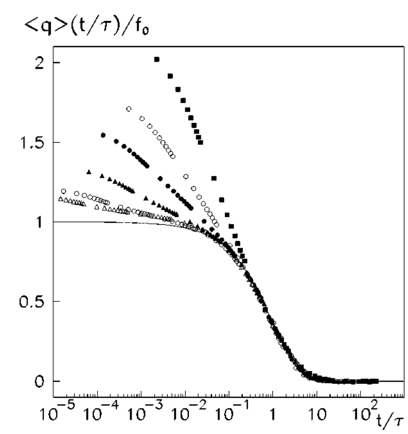

FIG. 4. The scaled relaxation functions of the self-overlap, $\langle q\rangle(t/\tau)/f_0$, as a function of the scaled time, t/τ, at the densities $\rho=0.54$, 0.59, 0.63, 0.66. 0.71 (from right to left). The continuous curve is a stretched exponential function with $\delta=0.71$.

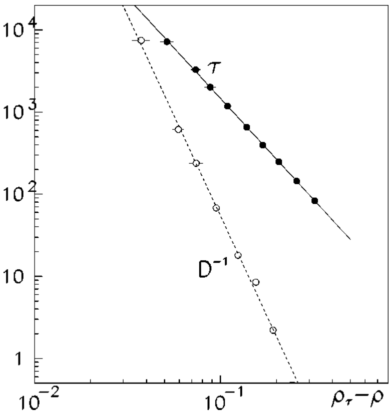

FIG. 5. The relaxation time, τ, and the inverse diffusion coefficient, D^{-1} (the empty circles in figure), are plotted as function of $\rho_\tau - \rho$. The curves are the power laws obtained as fitting functions.

$\simeq 0.93$ not depending on the density; and $\chi(t)$ tends to a plateau, which smoothly increases as a function of density. We suggest that this behavior might be due to the fact that there is only a few residual frustration on loops of length greater than 4, and frustration is too local to originate a slow dynamics.

A very different behavior is instead observed in the model with $r_{\max}=6$ (where the interactions evolve under the constraint that the number of frustrated loops of length 4 and 6 are independently kept constant). In Fig. 2, $\langle q\rangle(t)$ are plotted at different values of the density. At high density two step decays appear and the curves are well fitted at intermediate times by the forms predicted near the dynamical transition by the mode coupling theory (MCT) [2,8] (see Fig. 3). In Fig. 4, the scaled relaxation functions of the self-overlap, $\langle q\rangle(t/\tau)/f_0$, are plotted as function of the scaled time, t/τ. At long times the curves collapse onto a single master function, well fitted by a stretched exponential (the continuous curve in figure), and the relaxation time, τ, diverges as a power law, $(\rho_\tau-\rho)^{-\gamma_\tau}$, with $\rho_\tau \simeq 0.79\pm 0.02$ and $\gamma_\tau=4.9\pm 0.7$ (see Fig. 5).

The dynamical nonlinear susceptibility, $\chi(t)$, shown in Fig. 6, presents a maximum at a time, t^*, which we interpret as the relaxation time of the interactions: Until t^* the dynamical nonlinear susceptibility increases as if the environment were quenched, and only for $t>t^*$ the interactions evolve and $\chi(t)$ can decrease to the equilibrium value. A dynamical nonlinear susceptibility with a maximum is typical of glassy systems [9,10]. As in Lennard-Jones liquids we found that the value of the maximum, $\chi(t^*)$, which diverges in the p-spin model [9] as the dynamical transition is approached from above, has instead a maximum: We suggest that in the present case this behavior might due to the fact that the system becomes less and less frustrated as the density increases [11].

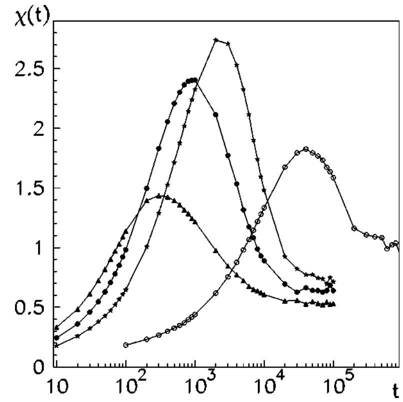

FIG. 6. The dynamical nonlinear susceptibility, $\chi(t)$, for $r_{\max}=6$ at the densities $\rho=0.48$, 0.54, 0.59, 0.069, (from left to right).

Finally we calculated the particle mean square displacement, $\langle \Delta r^2\rangle(t)=1/N_p\Sigma_i^{N_p}\langle(\mathbf{r}_i(t+t')-\mathbf{r}_i(t'))^2\rangle$, where $\mathbf{r}_i(t)$ is the position of the ith particle at the time t. At high density the mean square displacement is not linear at short time, and the diffusion coefficient, D, is calculated from the long time regime of the mean square displacement via the relation, $D=\lim_{t\to\infty}\langle\Delta r^2\rangle(t)/6t$. The diffusion coefficient, shown in Fig. 5, is well fitted by a power law, $(\rho_D-\rho)^{\gamma_D}$, with $\rho_D=0.80\pm 0.01$ and $\gamma_D=2.46\pm 0.19$. The critical density, ρ_D, obtained in this way coincides with the value, $\rho_\tau=0.79\pm 0.02$, where the relaxation time, τ, diverges; the exponent, γ_D, is instead not consistent with $\gamma_\tau=4.9\pm 0.7$.

In conclusions the properties of the annealed models, Eq. (2), strongly depend on the value of $r_{\max}$. In particular by increasing the degree of frustration a crossover from a liquidlike to a glassylike behavior is found. We suggest that the model with $r_{\max}=6$, where a dynamical glass transition is observed, in mean field might undergo a p-spin like transition with a 1-step replica symmetry breaking in the spin overlap distribution. Moreover it is reasonable to expect that, by further increasing the degree of frustration, the annealed partition function, Eq. (2), might tend to the quenched one, where a spin glasslike transition [4,12] and the development of a continuous replica symmetry breaking in the spin overlap distribution [14] is found, and a crossover from glassylike to spin glasslike behavior might be observed.

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[8] The β-correlator predicted by the MCT is given by $\Phi(t) = f_c + g(t/t_\sigma)$, where $g(t/t_\sigma)\propto(t/t_\sigma)^{-a}$ for $t_0 \ll t \ll t_\sigma$, and $g(t/t_\sigma)\propto-(t/t_\sigma)^{b}$ for $t_\sigma \ll t \ll \tau_\alpha$.

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[12] In the quenched FLG model the relaxation functions of the spin self-overlap were found to be well fitted by the function $ct^{-x}\exp(-(t/\tau)^{\delta})$, proposed by Olgielski for the Ising spin glass [13], and the dynamical nonlinear susceptibility to increase as function of time to a plateau value, which coincides with the static nonlinear susceptibility and diverges at the transition [5].

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