

## Glass transition in the quenched and annealed version of the frustrated lattice gas model

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In this paper we study the three-dimensional frustrated lattice gas model in the annealed version, where the disorder is allowed to evolve in time with a suitable kinetic constraint. Although the model does not exhibit any thermodynamic transition it shows a diverging peak at some characteristic time in the dynamical nonlinear susceptibility, similar to the results on the  $p$ -spin model in mean field and the Lennard-Jones mixture recently found by Donati *et al.* (e-print cond-mat/9905433). Comparing these results to those obtained in the model with quenched interactions, we conclude that the critical behavior of the dynamical susceptibility is reminiscent of the thermodynamic transition present in the quenched model, and signaled by the divergence of the static nonlinear susceptibility, suggesting therefore a similar mechanism also in supercooled glass-forming liquids.

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### I. INTRODUCTION

The study of glass forming systems and spin glasses has shown that these systems present a similar complex dynamical behavior. In both cases the relaxation time increases dramatically when the temperature is lowered; furthermore at temperatures lower than some temperature  $T^*$ , the relaxation functions are well fitted at long times by a stretched exponential function

$$f(t) = f_0 \exp\left\{-\left(\frac{t}{\tau_\alpha}\right)^\beta\right\}, \quad 0 < \beta < 1. \quad (1)$$

This similarity was further stressed by the observation that the dynamical equations of a class of mean field spin glass models, called  $p$ -spin glasses [1], are precisely equal to the mode coupling equations for supercooled liquids. The  $p$ -spin glasses are a generalization of the spin glass model, where spins interact via three or more body interactions.

Despite these analogies the connection in finite dimension between glass forming systems and spin glasses is not completely clear. As far as the static properties are concerned, spin glasses undergo a thermodynamic transition at a well defined temperature  $T_{SG}$ , where the nonlinear susceptibility diverges (a similar behavior is found also in the  $p$  spin in finite dimension [2]). The class of systems that show a transition of this kind contains systems with very different microscopic structures, but with two essential common characteristics, namely, the presence of competitive interactions (frustration) and of quenched disorder. On the other hand, glass formers are a class of systems where disorder is not originated by some fixed external variables, but is “self-generated” by the positions and orientation of particles. Differently from spin glasses, in glass forming liquids there is no sharp thermodynamic transition, characterized by the divergence of a thermodynamical quantity analogous to the nonlinear susceptibility in spin glasses. However Donati *et al.* [3] have recently introduced a time dependent nonlinear susceptibility both for spin models and for structural glasses: they have shown that in the mean field spherical model (where the mode coupling equations are exact), and in

a Lennard-Jones mixture studied by molecular dynamics simulation [4], the dynamical susceptibility exhibits a maximum at some characteristic time, and that this maximum diverges as the dynamical temperature  $T_D$  is approached from above. One may wonder whether the presence of this maximum is related somehow to the presence of “quasi-quenched” disorder self-generated in the liquid, resembling the divergence of the nonlinear susceptibility present in spin systems with quenched disorder. To shed some light on this problem in this paper we want to compare the properties of the frustrated lattice gas model, which has been recently introduced in the context of the glass transition [5], in two cases: when the disorder is quenched and when the disorder is self-generated.

In the quenched case the model is a spin glass diluted with lattice gas variable, that being constituted by diffusing particles is suited to study quantities such as the diffusion coefficient or the density autocorrelation functions, that are usually important in the study of liquids. This model exhibits in mean field [6] properties closely related to those of  $p$ -spin models. In three dimensions (3D), at low enough temperature, numerical simulations [7] show a behavior of the diffusion coefficient very similar to that experimentally observed in fragile liquids [8]. Moreover the model presents a continuous static transition where the fluctuations of the order parameter, which coincide with the nonlinear susceptibility, diverge. This property is absent in the infinite dimension  $p$ -spin models [3] and in supercooled liquids studied by molecular dynamics simulations, as Lennard-Jones binary mixtures [4].

Here we show the results obtained by studying the 3D frustrated lattice gas model in the annealed version, where the interactions are allowed to evolve with a kinetic constraint [10]. We find that the dynamical behavior fits quite well the behavior predicted by the mode coupling theory. It is also easy to show that the model does not present any thermodynamic transition, consequently there is no divergence in the nonlinear susceptibility. However the dynamical nonlinear susceptibility exhibits a maximum with a behavior similar to that found in the mean field  $p$ -spin model and in molecular dynamics simulation of Lennard-Jones mixture. We compare this behavior with the corresponding quantities

calculated in the quenched version and conclude that the thermodynamic transition, present in the quenched model and signaled by the divergence of the static susceptibility, manifests itself in the annealed model in the critical behavior of the dynamical susceptibility. This behavior seems a consequence of the fact at short enough time the interactions can be considered as quenched variables. Since the annealed model shows a behavior reminiscent of supercooled glass forming liquids, these results suggest that also in glass forming liquids the behavior of time dependent nonlinear susceptibility can be due to the presence of slow degree of freedom which acts for short time as quenched variables. Although the annealed lattice gas model does not show any thermodynamic transition, we cannot exclude that this is due to the absence of significant interactions: typically in a real system the dynamical constraint corresponds to some kind of interactions; in our case the static of the model is instead described by a trivial Hamiltonian, while the complex dynamics is due to the kinetic constraint.

In Sec. II we recall briefly the main results of the mode coupling theory for supercooled liquids; in Sec. III we introduce the dynamical nonlinear susceptibility as defined by Donati *et al.* Finally in Sect. IV we present the frustrated lattice gas model and the dynamical behavior observed by numerical simulations in the quenched (Sec. IV A) and in the annealed version (Sec. IV B).

## II. MODE COUPLING THEORY

In order to compare the dynamical behavior of the frustrated lattice gas with the predictions of the mode coupling theory (MCT) for supercooled liquids [9] we recall briefly the results of this theory. The equations of motion of the normalized spatial Fourier transform of the density autocorrelation functions  $\Phi_q(t)$  are evaluated under suitable approximations and a dynamical transition, considered as an idealization of the glass transition, is observed: at high temperature the solutions  $\Phi_q(t)$  vanish at long time (liquid phase); at temperatures below a certain critical value  $T_{\text{MCT}}$  solutions with a nonzero long time limit  $f_q$  (called Debye-Waller factor) appear (glass phase). This transition is due to the nonlinearity of the equations, and no thermodynamic phase transition is present.

Let us introduce some important quantities: the exponent parameter  $0.5 \leq \lambda < 1$ , that is a constant depending only on the system, and the separation parameter  $\sigma$ , that is proportional to  $x - x_c$ , where  $x$  is the external control parameter (density or temperature) and  $x_c$  is the critical value ( $\sigma$  is chosen positive in the glass phase). Via the transcendental equation

$$\frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)} = \lambda, \quad (2)$$

the exponent  $\lambda$  determines two exponents  $0 < a < 0.5$  and  $0 < b \leq 1$ , that rule the relaxation of the system near the critical point.

The MCT predicts that in the  $\beta$  regime, near the dynamical transition, the correlators can be written as

$$\Phi_q(t) = f_q^c + h_q c_\sigma g_\pm(t/t_\sigma), \quad \text{for } t_0 \ll t \ll \tau_\alpha, \quad (3)$$

where  $c_\sigma = \sqrt{|\sigma|}$  and  $\pm$  refers, respectively, to the glass and liquid phase. The exponent  $a$  fixes the short time behavior,  $g_\pm(t/t_\sigma) = (t/t_\sigma)^{-a}$  for  $t_0 \ll t \ll t_\sigma$ , while for  $t_\sigma \ll t \ll \tau_\alpha$  one has a constant in the glass phase  $g_+(t/t_\sigma) = (1-\lambda)^{1/2}$ , and the so called von Schweidler law in the liquid phase  $g_-(t/t_\sigma) = -B(t/t_\sigma)^b$ . Here two time scales, diverging as the critical point is approached from above, appear

$$t_\sigma = t_0 |\sigma|^{-\delta}, \quad \delta = \frac{1}{2a}; \quad (4)$$

$$\tau_\alpha = t_0 B^{-1/b} |\sigma|^{-\gamma}, \quad \gamma = \frac{1}{2a} + \frac{1}{2b}; \quad (5)$$

and  $t_0$  is a microscopic time characteristic of molecules motion.

Furthermore, in the liquid phase, the theory predicts the following scaling law for the  $\alpha$  relaxation ( $t \gg \tau_\alpha$ ):

$$\Phi_q(t) = \tilde{\Phi}_q\left(\frac{t}{\tau_\alpha}\right); \quad (6)$$

where the master curve  $\tilde{\Phi}_q(t/\tau_\alpha)$  is well fitted by a stretched exponential of the form (1), with  $0 < \beta < 1$  depending on the particular correlator, but not on the temperature. This functional form usually fits the experiments as well.

In order to test the predictions of the MCT in the  $\beta$  regime, Gleim and Kob [11] have introduced the following quantity:

$$R_q(t) = \frac{\Phi_q(t) - \Phi_q(t')}{\Phi_q(t'') - \Phi_q(t')}, \quad (7)$$

where  $t'$  and  $t''$  are arbitrary times in the  $\beta$  regime ( $t' \neq t''$ ). From Eq. (3) we can see that, if  $\Phi_q(t)$  is in agreement with the leading-order prediction of the theory, then  $R_q(t)$  must be independent on  $q$  in the  $\beta$  regime.

## III. DYNAMICAL NONLINEAR SUSCEPTIBILITY

Donati *et al.* [3] have recently defined a dynamical nonlinear susceptibility both for spin models and for structural glasses. They have shown that in the mean field  $p$ -spin spherical models (where the mode coupling equations are exact) there is a characteristic time where the dynamical susceptibility has a maximum, and that this maximum diverges as the dynamical temperature  $T_D$  is approached from above.

The Hamiltonian of the  $p$ -spin model is

$$H = \sum_{i_1 < \dots < i_p} J_{i_1 \dots i_p} S_{i_1} \dots S_{i_p}, \quad (8)$$

where  $p \geq 3$ , the couplings  $J_{i_1 \dots i_p}$  are Gaussian with zero mean and variance  $1/N^{p-1}$ , and the spins are real variables, with the global constraint  $\sum_{i=1}^N S_i^2 \equiv N$ , where  $N$  is the number of spins. The dynamical nonlinear susceptibility  $\chi(t)$  is defined by

$$\chi(t) = \beta N [\langle q(t)^2 \rangle - \langle q(t) \rangle^2], \quad (9)$$

where  $q(t) = (1/N) \sum_i S_i(t') S_i(t'+t)$  is the overlap between the states at times  $t'$  and  $t'+t$ . Solving the equation of motion for  $\chi(t)$  at temperature higher than  $T_D$ , they find that  $\chi(t)$  displays a maximum as a function of time,  $\chi(t^*)$ , which is shifted to larger times  $t^*$  as  $T$  approaches  $T_D$  from above and increases as a power law  $\chi(t^*) \propto (T - T_D)^{-\alpha}$ .

A similar behavior has also been found in molecular dynamics simulation performed for a Lennard-Jones mixture.

#### IV. FRUSTRATED LATTICE GAS MODEL

##### A. The quenched model

Recently a lattice model, which has mean field properties closely related to those of  $p$ -spin models, has been introduced [5] in connection with the glass transition. This model is a diluted spin glass, which, being constituted by diffusing particles, is suited to study quantities such as the diffusion coefficient, or the density autocorrelation functions, that are usually important in the study of liquids. The Hamiltonian of the model is

$$-\beta H = J \sum_{\langle ij \rangle} (\epsilon_{ij} S_i S_j - 1) n_i n_j + \mu \sum_i n_i, \quad (10)$$

where  $S_i = \pm 1$  are Ising spins,  $n_i = 0, 1$  are occupation variables, and  $\epsilon_{ij} = \pm 1$  are quenched and disordered interactions.

This model reproduces the Ising spin glass in the limit  $\mu \rightarrow \infty$  (all sites occupied,  $n_i \equiv 1$ ). In the other limit,  $J \rightarrow \infty$ , the model describes a frustrated lattice gas with properties recalling those of a ‘‘frustrated’’ liquid. In fact the first term of Hamiltonian (10) implies that two nearest neighbor sites can be freely occupied only if their spin variables satisfy the interaction, that is if  $\epsilon_{ij} S_i S_j = 1$ , otherwise they feel a strong repulsion.

To make the connection with a liquid, we note that the internal degree of freedom  $S_i$  may represent, for example, internal orientation of a particle with nonsymmetric shape. Two particles can be nearest neighbors only if the relative orientation is appropriate, otherwise they have to move apart. Since in a frustrated loop the spins cannot satisfy all 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.

Another possible interpretation of the model is that  $n_i$  is the occupation variable of the  $i$ th cell and  $S_i$  indicates the position of the center of mass of the particle inside the cell.  $S_i$  can in principle assume many different values corresponding to the coordinates of the center of mass inside the cell. The interaction should take into account that not all pair of internal degree of freedom in two neighbors cells are allowed. In the frustrated lattice gas model for simplicity we drastically reduce the internal degree of freedom to only two values ( $S_i = \pm 1$ ) and introduce the interaction  $\epsilon_{ij} = \pm 1$  between two neighbor spin variables to mimic the local disorder of the medium. In the first version of the model we assume that the local disorders are quenched.

In the case  $J = \infty$  the model has a maximum density  $\rho_{\max} \approx 0.68$ . It has been shown that there exists some density

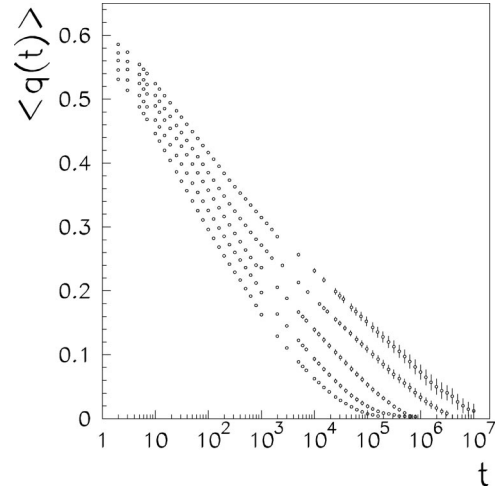


FIG. 1. Relaxation functions of the self-overlap in the quenched model, for a system of size  $16^3$  and densities  $\rho = 0.58, 0.59, 0.60, 0.61, 0.62$ .

$\rho_c \approx 0.62$ , where the system has a transition of the type of 3d  $p$ -spin model [12], with a divergence of the static nonlinear susceptibility

$$\chi_{\text{SG}} = \frac{1}{N} \sum_{ij} [\langle S_i n_i S_j n_j \rangle^2], \quad (11)$$

where the average  $\langle \dots \rangle$  is over the Boltzmann measure, while the average  $[\dots]$  is over the disorder configurations  $\{\epsilon_{ij}\}$ .

Here we show the results for the relaxation of the self-overlap, which is defined as

$$q(t) = \frac{1}{N} \sum_i S_i(t') n_i(t') S_i(t'+t) n_i(t'+t), \quad (12)$$

and for the dynamical susceptibility

$$\chi(t) = N [\langle q(t)^2 \rangle - \langle q(t) \rangle^2], \quad (13)$$

where the average  $\langle \dots \rangle$  is done on the reference time  $t'$ . In Fig. 1 it is shown the relaxation functions  $\langle q(t) \rangle$  for a system of size  $16^3$  for densities between  $\rho = 0.58$  and  $0.62$ . Each curve is obtained averaging over a time interval for  $t'$  of  $6 \times 10^6 - 8 \times 10^7$  Monte Carlo steps, and finally averaging the results over 16 realizations of the disorder. Note that there is no sign of a two step relaxation. The long time tail of the functions can be well fitted by a stretched exponential form, with an exponent  $\beta$  strongly dependent on the density, which tends to very low values  $\beta \approx 0.2$  at high density. In Fig. 2 it is shown the dynamical susceptibility  $\chi(t)$  for the same size and values of density of Fig. 1. Note that  $\chi(t)$  grows monotonically and has no maximum at finite time. The asymptotic value  $\chi(\infty)$  corresponds to the static susceptibility (11), and therefore has a divergence at the density  $\rho_c \approx 0.62$ .

##### B. The annealed model

We have studied the frustrated lattice gas model (10) in the case where the interactions  $\epsilon_{ij} = \pm 1$  are annealed. When we evaluate the partition function of the model, we must

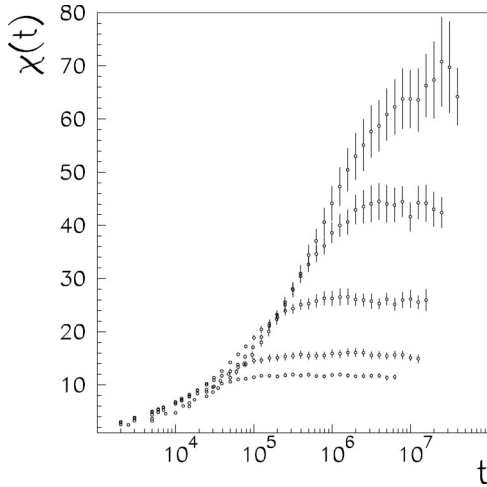


FIG. 2. Dynamical susceptibility in the quenched model, for the same system size and densities of Fig. 1.

consider in this case not only the  $S_i$  and  $n_i$ , but also the  $\epsilon_{ij}$  as dynamical variables. Thus, summing over the  $\epsilon_{ij}$  and  $S_i$  we obtain, apart from an irrelevant factor,  $Z = \sum_{\{n_i, S_i, \epsilon_{ij}\}} e^{-\beta H} = \sum_{\{n_i\}} e^{-\beta H_{\text{eff}}}$ , where

$$-\beta H_{\text{eff}} = -K \sum_{\langle ij \rangle} n_i n_j + \mu \sum_i n_i, \quad (14)$$

and  $K = -\ln[(1 + e^{-2J})/2]$ . Therefore the static properties of the model are equal to those of a lattice gas with a repulsion between nearest neighbor particles, and with no correlation between spins,  $\langle S_i S_j \rangle = \delta_{ij}$ . With the change of variables  $n_i = \frac{1}{2}(1 + \sigma_i)$ , where  $\sigma_i = \pm 1$  are Ising spins, this Hamiltonian can be written as the Hamiltonian of an antiferromagnetic Ising model with an effective temperature  $T_{\text{eff}} = 4K^{-1}$ , which is always greater than the critical temperature of the 3D antiferromagnetic Ising model  $T_c \approx 4.5$ . Therefore we can conclude that the model (14), and then also the model (10) with annealed interactions, does not present any thermodynamic transition. In the following we consider always the model with  $J = \infty$ .

We assume a dynamics for the variables  $\epsilon_{ij}$  with a kinetic constraint, namely,  $\epsilon_{ij}$  can change its state only if the sites  $i$  and  $j$ , and all their nearest neighbors, are empty; in this way the accessible states to a given particle may change only if a wide enough region of the system around it rearranges itself. We expect that, as the temperature decreases, the disorder due to the local environment changes so slowly that the interactions behave more and more as frozen playing the role of ‘‘self-induced quenched’’ variables.

In order to generate an equilibrium configuration at a given density we simulate the model without any dynamical constraint. In this case we can thermalize the system even at high density. Once an equilibrium configuration is obtained, we consider a diffusive dynamics for the particles while the interactions evolve with the kinetic constraint, as described before. In conclusion the simulations are done in the following way.

(1) One starts from an equilibrium configuration obtained at some density  $\rho$ .

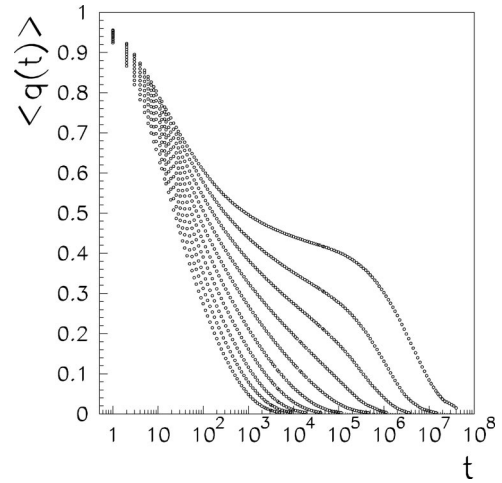


FIG. 3. Relaxation functions of the self-overlap in the annealed model, for a system of size  $16^3$  and densities  $\rho = 0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.60, 0.61$ .

(2) At each step of dynamics an interaction  $\epsilon_{ij}$  is randomly chosen and is changed if the sites  $i$  and  $j$ , and all their nearest neighbors, are empty.

(3) A particle (occupied site) on the lattice, one of the coordinate directions, and a final state of the spin  $S_i$  are randomly chosen.

(4) One tries to move the particle to the nearest neighbor site in the chosen direction. The particle can move if two conditions are both satisfied. First, the destination site must be empty. Second, the spins of the particles that are nearest neighbors of the destination site, must satisfy the interaction with the spin of the chosen particle. If the particle cannot move in the chosen site, then the move is rejected.

(5) The clock advances one unit of time.

During this dynamics we have evaluated relaxation functions and dynamic nonlinear susceptibility. Note that as density grows, the relaxation time gets longer and longer, and gets longer than our observation time (which is between  $10^7$  and  $10^8$  for a system of size  $16^3$ ) at a density approximately  $\rho \approx 0.63$ .

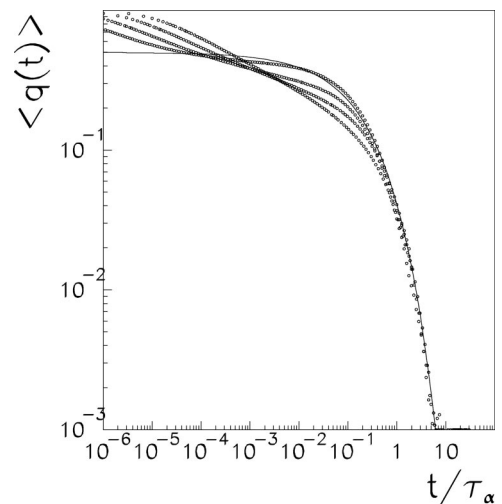


FIG. 4. Time temperature superposition principle for the relaxation functions of the self-overlap, for densities  $\rho = 0.58, 0.59, 0.60, 0.61$ . The fitting function is a stretched exponential with exponent  $\beta = 0.5$ .

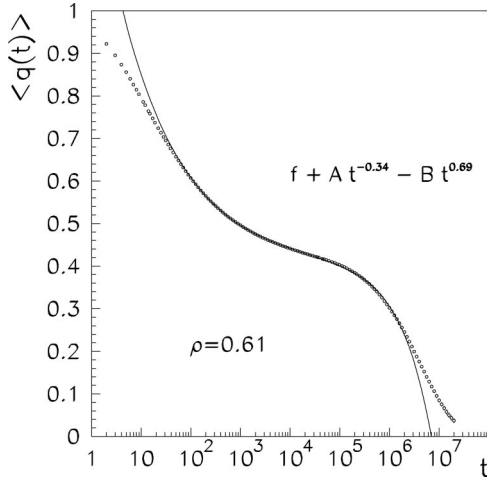


FIG. 5. Fit of the intermediate time part of the relaxation function of the self-overlap, for density  $\rho=0.61$ , with the fitting function  $f + A t^{-a} - B t^b$ , where the fitting parameters are  $f$ ,  $A$ ,  $B$ , and  $\lambda$ , and  $a$  and  $b$  are given by the relation (2).

In Fig. 3 we show the relaxation functions of the self-overlap (12), for a system of size  $16^3$ , for various densities between  $\rho=0.52$  and  $0.61$ . Each curve is obtained averaging over a time interval for  $t'$  of  $3 \times 10^6 - 10^8$  Monte Carlo steps. Observe that for high density the relaxation functions clearly develop a two step relaxation, signaling the existence of two well separated time scales in the system. We interpret the first short time decay of the relaxation functions as due to the motion of the particles in the frozen environment, which on this time scales appear as quenched, while the second decay is due to the evolution of environment, and final relaxation to equilibrium of the system. The long time tail of the relaxation functions is well fitted by a stretched exponential form (1), where the exponent  $\beta$  depends very weakly from the temperature (it is constant within the errors) and ranges between  $\beta=0.4$  and  $\beta=0.6$ . In Fig. 4 we show the time-temperature superposition of the relaxation functions of the overlap, for densities between  $\rho=0.58$  and  $\rho=0.61$ . We tried to fit the intermediate time part, corresponding to the plateau, of the relaxation function of the overlap for density

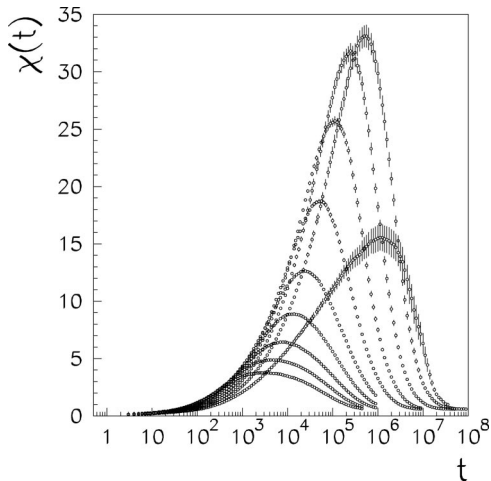


FIG. 6. Dynamical susceptibility in the annealed model, for the same system size and densities of Fig. 3.

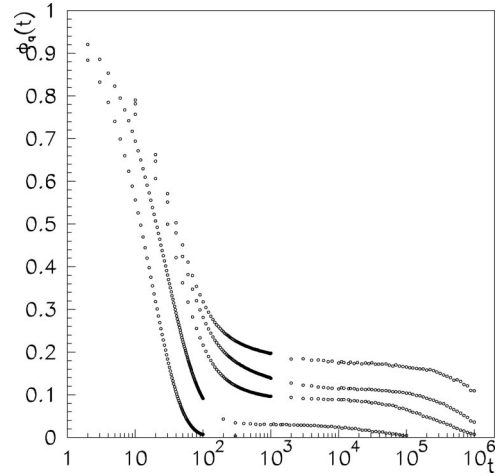


FIG. 7. Correlation functions of the density fluctuations  $\Phi_q(t)$  for  $q = (\pi/4, 0, 0)$  at densities (from bottom to top)  $\rho = 0.380, 0.490, 0.543, 0.584, 0.602$ .

$\rho=0.61$ , with the function predicted by the MCT (in a simplified form)

$$\langle q(t) \rangle = f + A t^{-a} - B t^b, \quad (15)$$

where the fitting parameters are  $f$ ,  $A$ ,  $B$ , and  $\lambda$ , while  $a$  and  $b$  are given by the relation (2). The result is shown in Fig. 5, where the full line is the fitting curve with  $a = 0.339 \pm 0.002$  and  $b = 0.69 \pm 0.01$ .

In Fig. 6 we show the dynamical nonlinear susceptibility (13) for the same size and values of the density of Fig. 3. It has the same behavior of the  $p$ -spin model in mean field and of the molecular dynamics simulation of the Lennard-Jones binary mixture [3], namely, a maximum  $\chi(t^*)$  that seems to diverge together with the time of the maximum  $t^*$ , when the density grows. For the highest density, the maximum of  $\chi(t)$  decreases, possibly due to finite size effects, too short observation time, or a change in the dynamics above some critical density. This fact is observed also in MD simulations of Lennard-Jones liquids [4]. We obtain that the maximum  $\chi(t^*)$  as a function of the density can be fitted quite well

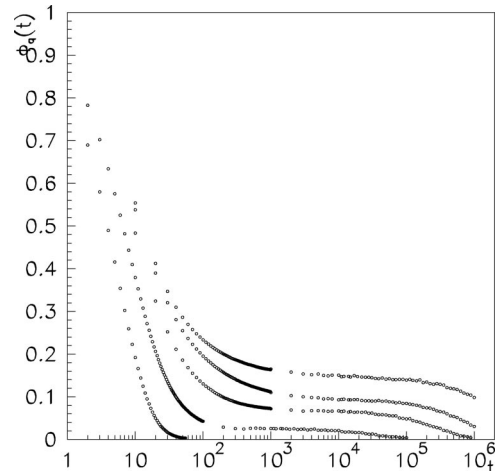


FIG. 8. Correlation functions of the density fluctuations  $\Phi_q(t)$  for  $q = (\pi/2, 0, 0)$  at densities (from bottom to top)  $\rho = 0.380, 0.490, 0.543, 0.584, 0.602$ .

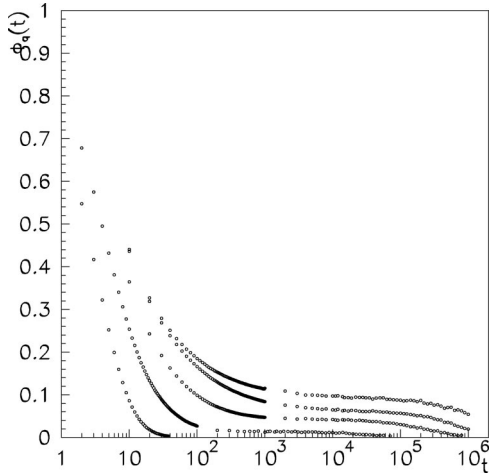


FIG. 9. Correlation functions of the density fluctuations  $\Phi_q(t)$  for  $\mathbf{q}=(\pi,0,0)$  at densities (from bottom to top)  $\rho=0.380, 0.490, 0.543, 0.584, 0.602$ .

(taking out the last three points, where presumably a rounding of the divergence takes place) by the power law  $\chi(t^*) \propto (\rho_c - \rho)^{-\alpha}$ , with  $\rho_c = 0.66 \pm 0.01$  and  $\alpha = 3.6 \pm 0.2$ . At very long times  $\chi(t)$  decays to the equilibrium value, which is simply  $\chi(\infty) = \rho^2$ .

To make a more direct comparison with MCT, we have evaluated, on a cubic lattice of size  $8^3$ , the autocorrelation functions of the density fluctuations

$$\Phi_q(t) = \frac{\langle \delta\rho_q(t'+t)\delta\rho_q(t') \rangle}{\langle |\delta\rho_q|^2 \rangle}, \quad (16)$$

where the average  $\langle \dots \rangle$  is performed on time  $t'$ , the density fluctuation of wave number  $\mathbf{q}$  is defined by  $\delta\rho_q = \rho_q - \langle \rho_q \rangle$ , and

$$\rho_q(t) = \sum_{i=1}^n e^{-i\mathbf{q} \cdot \mathbf{r}_i(t)}, \quad (17)$$

where  $\mathbf{r}_i(t)$  is the position of the  $i$ th particle at time  $t$  and  $n$  is the particle number.

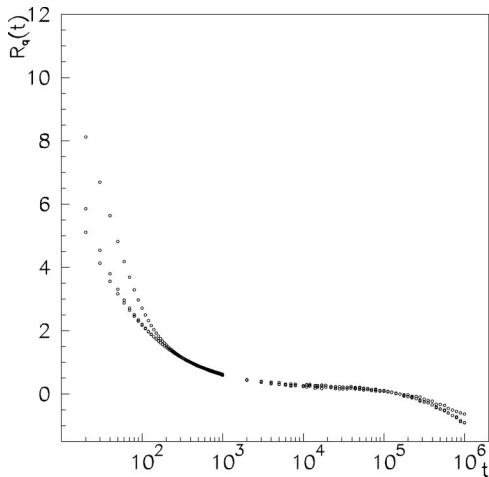


FIG. 10.  $R_q(t)$  for  $\mathbf{q}=(\pi/4,0,0), (\pi/2,0,0),$  and  $(\pi,0,0)$  at density  $\rho=0.584$ .

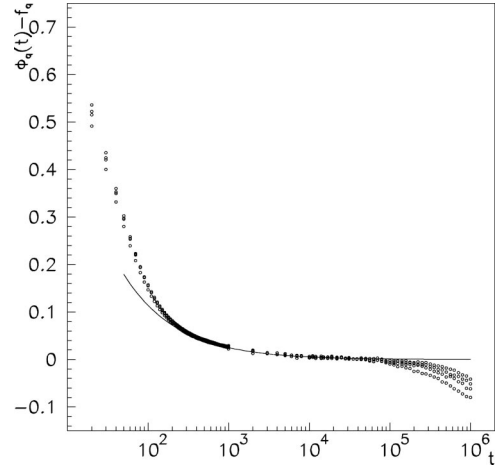


FIG. 11.  $[\Phi_q - f_q]$  as function of time  $t$  for  $\mathbf{q}=(\pi/4,0,0)$  at  $\rho=0.548, 0.573, 0.602, 0.615$ . The full line is the power law  $(t/3.6)^{-0.66}$ .

Because of periodic conditions the allowable values of  $\mathbf{q}$  on a cubic lattice are of the form

$$\mathbf{q} = \frac{2\pi}{L}(n_x, n_y, n_z), \quad (18)$$

where  $n_x, n_y, n_z = 1 \dots L/2$  are integer values.

In Figs. 7–9 we show the results obtained at densities between  $\rho=0.380$  and  $\rho=0.602$ , respectively, for  $\mathbf{q}=(\pi/4,0,0), (\pi/2,0,0),$  and  $(\pi,0,0)$ . Each curve is obtained averaging over a time interval for  $t'$  of  $10^6$ – $10^7$  steps and finally averaging the results obtained by 32–128 different simulations. As we can see in figures, at low density the autocorrelation functions relax to zero with a one step decay; on the other hand, as the density increases we can recognize the two-step decay characteristic of glass forming systems.

As we have said in Sec. II, if  $\Phi_q(t)$  satisfies the prediction of the MCT,  $R_q(t)$  (7) must be independent on  $q$  in the  $\beta$  regime. We have evaluated  $R_q(t)$  (with  $t'' \approx 400$  and  $t' \approx 1.6 \times 10^5$ ) at some densities for all values of  $q$  considered here and we have obtained that  $R_q(t)$  is independent on  $q$  on

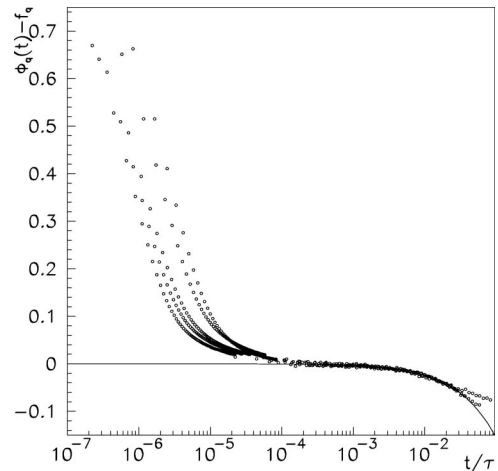


FIG. 12.  $[\Phi_q - f_q]$  as function of  $t/\tau$  for  $\mathbf{q}=(\pi/4,0,0)$  at  $\rho=0.548, 0.573, 0.602, 0.615, 0.625$ . The full line is the von Schweidler law  $-(t/\tau)^{0.80}$ .

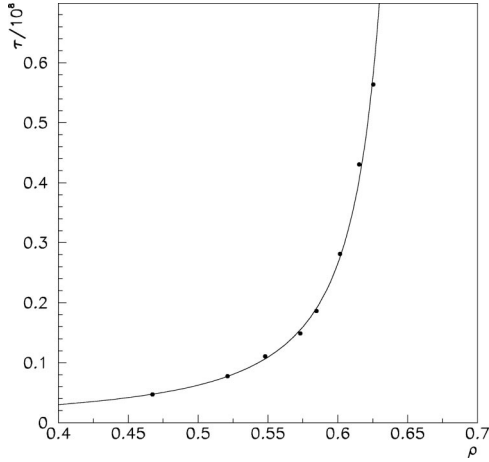


FIG. 13. The relaxation time  $\tau$  as function of density  $\rho$ . The full line is the power law  $(0.66 - \rho)^{-1.5}$ .

a large time interval (see Fig. 10). In agreement with this result we find that, after the initial transient, the correlators  $\Phi_q(t)$  are well fitted by a power law

$$f_q + h_q \left( \frac{t}{t_0} \right)^{-a} \quad (19)$$

and, in the intermediate time region, by a von Schweidler law

$$f_q - h_q \left( \frac{t}{\tau} \right)^b, \quad (20)$$

where the exponents  $a$  and  $b$  are independent on  $q$ .

In Figs. 11 and 12 we show  $[\Phi_q(t) - f_q]$  as function, respectively, of  $t$  and  $t/\tau$  for  $\mathbf{q} = (\pi/4, 0, 0)$  at different values of densities. As we can see in figures the curves scale for all values of density considered here and the data are in good agreement, respectively, with the power law  $(t/t_0)^a$  (with  $a = 0.66 \pm 0.11$  and  $t_0 = 3.6 \pm 3.0$ ) and the von Schweidler law  $-(t/\tau)^b$  (with  $b = 0.80 \pm 0.13$ ). The relaxation time  $\tau$ , obtained as fitting parameter from Eq. (20), is an increasing function of density, well represented by a power law  $(\rho_c - \rho)^{-\gamma}$ , with  $\rho_c = 0.66 \pm 0.03$  and  $\gamma = 1.5 \pm 0.2$  (see Fig. 13). However, the values of the exponents  $a$  and  $b$  obtained in this case do not satisfy the relation (2) and are not in agreement with the exponents obtained for  $\langle q(t) \rangle$ .

In Fig. 14 we show the correlators  $\Phi_q(t)$  as functions of the rescaled times  $\tilde{t} = t/\tau_\alpha$ ; as we can see, the curves coincide at large  $\tilde{t}$ , for all values of density considered here, with a common master curve  $\tilde{\Phi}_q$ , well fitted by a stretched exponential function [for  $\mathbf{q} = (\pi/4, 0, 0)$  we obtain  $\beta \approx 0.45$ ]. This result is consistent with the predictions of the MCT concerning the  $\alpha$  relaxation.

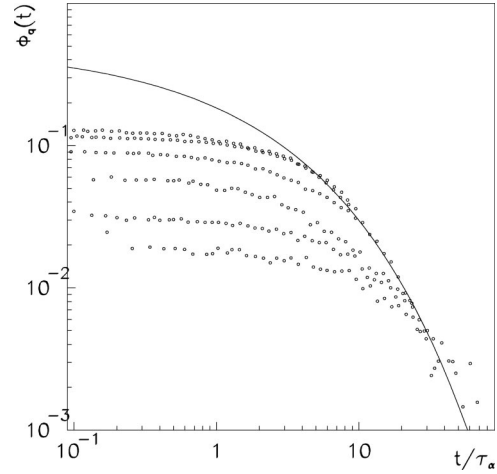


FIG. 14.  $\Phi_q$  as function of  $t/\tau_\alpha$  for  $\mathbf{q} = (\pi/4, 0, 0)$  at  $\rho = 0.467, 0.490, 0.521, 0.543, 0.573, 0.584$ . The full line is the stretched exponential function  $e^{-(t/\tau_\alpha)^{0.45}}$ .

Finally as the density grows the equilibrium system smoothly evolves towards an “ordered” state, analogous to the crystal state (the system at high enough density can reach the equilibrium state only if frustration is reduced). As a consequence of this fact, the similarity between the annealed model and a supercooled glass forming liquid fails at high density.

## V. CONCLUSIONS

The frustrated lattice gas model in the quenched version presents a thermodynamic transition at a critical density, where the static nonlinear susceptibility diverges. The annealed model, which does not present any thermodynamic transition, consequently does not show any critical behavior of the static susceptibility; on the other hand we observe an “apparent” divergence of the dynamical susceptibility at a value of density  $\rho_c$  (where the structural relaxation time also diverges). We suggest that this behavior is due to the fact that at short enough time the disorder can be considered as quenched. Moreover the similarity between the annealed model and the supercooled glass forming liquids suggests that also in these systems a similar mechanism may be responsible for the critical behavior of the dynamical susceptibility, and one might speculate that if one could in special systems freeze some degree of freedom one could find a behavior similar to systems with quenched disorder.

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