Dynamics of the frustrated Ising lattice gas

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The dynamical properties of a three-dimensional model glass, the frustrated Ising lattice gas (FILG), are studied by Monte Carlo simulations. We present results of compression experiments, where the chemical potential is either slowly or abruptly changed, as well as simulations at constant density. One time quantities like density and two time quantities like correlations, responses, and mean square displacements are measured, and the departure from equilibrium clearly characterized. The aging scenario, particularly in the case of density autocorrelations, is reminiscent of spin glass phenomenology with violations of the fluctuation-dissipation theorem, typical of systems with one replica symmetry breaking. The FILG, as a valid on-lattice model of structural glasses, can be described with tools developed in spin glass theory and, being a finite-dimensional model, can open the way for a systematic study of activated processes in glasses.

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I. INTRODUCTION

Upon cooling below the melting point, liquids may either crystallize or enter a super cooled regime. In the latter case, as the glass transition temperature T_g is approached, molecular motion becomes slower and slower and the viscosity increases enormously. The relaxation time increases by several orders of magnitude, and for all practical purposes the system remains out of equilibrium. Although mechanically responding as a solid, structural relaxation is still present, slowing down as the system ages. The response to a perturbation applied at a particular time t_w will persist for very long times (long term memory), preventing the system from reaching equilibrium. While the system ages, one time quantities tend asymptotically to their equilibrium values, while two time quantities depend explicitly both on the observation time and on the time when the perturbation was applied: time translation invariance is broken, which is a manifestation of history dependence. Upon cooling, the system is trapped on long lived metastable states which depend on the cooling rate, eventually escaping as a result of activated processes. This complex glassy dynamics is reflected in several characteristic features, as nonexponential relaxation, breakdown of fluctuation-dissipation relations, etc., and there is a widespread believe that the underlying rugged energy landscape plays a fundamental role on the dynamics [1]. Many aspects related to the structural glass transition and the nature of the glassy phase are still poorly understood [2,3], as a consequence of the inherent complexity of the underlying physics and the corresponding lack of a simple but nontrivial model. Only recently has some analytical progress been made with classic models based on Lennard-Jones or soft sphere potential [4] which, on the other hand, have been extensively studied via molecular dynamics simulations [5]. Meanwhile, in the field of spin glasses, disordered magnetic systems which share many physical properties with structural glasses, a reasonable theoretical understanding of the basic physics has been achieved at least at the mean field level [6,7]. Recently it was found that equations describing dynamical correlation functions of a kind of mean field spin glasses simplify, above the transition, to the single equation of the mode coupling theory of supercooled liquids [8]. In particular, several results point out that these models (e.g., the *p*-spin model) with one step of replica symmetry breaking and structural glasses are in the same universality class [9,10], indicating a deeper analogy between the physics of spin glasses and structural glasses than previously thought. Nevertheless, it is still a matter of debate to what extent this analogy can be pushed forward. Some important differences between these two kinds of systems are evident: while a defining feature of spin glasses is the quenched disorder and frustration, no obvious quench disorder is present in structural glasses. Several models with frustration but no disorder were recently studied [11]. Another important difference is the fact that dynamical variables in a spin glass are localized in space, and do not diffuse like the molecules in a supercooled liquid. We would like to have at hand a simple, yet nontrivial, microscopic model of supercooled liquids in which the fruitful techniques developed in spin glass theory could be applied and possibly extended to finite dimension. Moreover, mode coupling theory and mean field models in general do not describe activated processes, which are responsible for some important characteristics of the glass phase, like, e.g., the cooling rate dependence of the asymptotic state. There are some other very simple models with kinetic constraints which reproduce the glassy phenomenology [12,13] quite well, but, being essentially dynamical, they are hard to study with analytical techniques.

In this paper we describe salient dynamical features of a Hamiltonian lattice model of structural glasses, the frustrated Ising lattice gas (FILG). The interesting properties revealed by the model rest on an interplay between two different kinds of degrees of freedom: diffusive particles or transla-

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tional degrees of freedom, and internal or orientational degrees of freedom. We present results of Monte Carlo simulations of one and two time quantities, like density relaxation, density-density correlations and responses, correlations and responses of internal degrees of freedom, mean square displacements of the particles, and compression experiments. This three-dimensional model may serve as a numerical laboratory to perform a systematic study of the role played by activated processes on the long time dynamics of glass formers, a feature that is missing from mean field approximations.

The paper is organized as follows. In Sec. II, we review the essential results both from equilibrium and out of equilibrium dynamics for the FILG. In Sec. III, results for slowly varying chemical potentials are presented and compared with the case where a sudden quench is performed, while in Sec. IV the breakdown of the fluctuation-dissipation theorem in this model is analyzed. Finally, in Sec. V, we present some conclusions and discuss some open questions.

II. FRUSTRATED ISING LATTICE GAS

The FILG [14] is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} (\varepsilon_{ij} S_i S_j - 1) n_i n_j - \mu \sum_i n_i. \quad (1)$$

The dynamical variables $n_i = 0,1 (i = 1, \ldots, N)$ are local densities or site occupations. S_i represent internal degrees of freedom, e.g., rotational ones. Although molecules in glass forming liquids may assume several spatial orientations, here we take the simpler case of only two possibilities, $S_i = \pm 1$. The usually complex spatial structure of these molecules is in part responsible for the geometric constraints, imposed by the neighborhood, on their translational and rotational dynamics. This hindrance effect is mimicked by the quenched random variables $\varepsilon_{ij} = \pm 1$. When $J \to \infty$, in order to minimize $\mathcal{H}$, either the spins should satisfy the bond ε_{ij} or at least one of the sites i or j must be empty. In this limit, the (site) frustrated percolation [14] model is recovered, where no frustrated link can be fully occupied, implying that any frustrated loop in the lattice will have a hole and then $\rho < 1$, preventing the system from reaching the close packed configuration.

The equilibrium properties of the three-dimensional (3D) model were studied in Ref. [15] for $T = 1$ and $J = 10$, which corresponds in practice to the frustrated percolation limit. In the low density regime ($\mu \lesssim 0.75$) the behavior is liquidlike, time correlation functions decay exponentially, equilibration is quickly achieved, and the particles mean squared displacement grows linearly with time, a simple diffusion scenario since particles hardly feel any constraint in their mobility. At $\mu \approx 0.75$ there is a percolation transition, the corresponding density being $\rho \approx 0.38$. This first transition manifests itself dynamically in the onset of two different relaxation regimes in the correlation functions, a fast exponential relaxation at short times and a slow, stretched exponential relaxation at longer times. While for intermediate times the diffusion is anomalous, for longer times it is linear, with the diffusion coefficient becoming smaller as the density grows with growing chemical potential (or equivalently, with lowering

temperature). A second transition appears for $\mu_c \approx 5.5$, corresponding to a density $\rho_c \approx 0.67$. This is a glass transition at which the relaxation times diverge and the diffusion constant goes to zero. In the FILG the structural manifestation of this transition is the presence of a *frozen* percolating cluster. This transition corresponds to the dynamical one in mean field p-spin or Potts glasses or the ideal glass transition in the mode coupling theory. Scarpetta *et al* [16] studied an equivalent, nonlocal version of the FILG (site frustrated percolation) in two-dimensions, finding a behavior similar to the 3D FILG, the main difference being the (Arrhenius) dynamical singularity occurring at zero temperature. It was also found in Ref. [15] that the spin glass susceptibility χ_{SG}, associated with the internal degrees of freedom of occupied sites, diverges at the same value of μ where a glass transition takes place. This is a thermodynamic spin glass transition associated with the freezing of internal degrees of freedom. On the other hand, the compressibility associated with the density variables does not present a critical behavior but only a maximum, as observed in many glass formers. In view of this behavior one could ask whether a suitably defined nonlinear compressibility should diverge at the glass transition. This should indicate the thermodynamic character of the glass transition in this model. A nonlinear compressibility, $\kappa_{SG} = N(\langle q_n^2 \rangle - \langle q_n \rangle^2)$, can be introduced with $q_n = N^{-1} \Sigma_i n_i^1 n_i^2$, where 1 and 2 label two real replicas of the system. One could think that in this quantity, associated with fluctuations of an Edwards-Anderson-like order parameter involving only density variables, a divergence analogous to the one present in χ_{SG} might be detected. This quantity was measured [17], but no evidence of critical behavior was found near μ_c: κ_{SG} attains a plateau that seems to be roughly sample and size independent. The fact that the spin variables present a thermodynamic transition while the particles do not points once more to the purely dynamical character of the glass transition. Of course, a thermodynamic transition may be present at a lower temperature (or a higher chemical potential) corresponding to the Kauzmann T_K and associated with a configurational entropy collapse, but this remains an open question in this model which deserves further study.

At a mean field level, equilibrium properties have been studied in closely related models [18]. For large μ all sites are occupied and the behavior corresponds to the Sherrington-Kirkpatrick model, with a continuous spin glass transition. Upon decreasing μ one reaches a tricritical point, below which the transition is first order. In this region, analogously to other first order transition models like the p spin and the Potts glass [19], above the critical temperature there is a dynamical transition where metastable states first appear [18]. We still do not know to what extent this scenario remains valid in finite dimensions.

A characteristic feature of the out of equilibrium dynamics of glassy systems is aging [20]. Slow aging dynamics is present in the FILG both in density-density two time correlations as well as in correlations of the internal degrees of freedom [21] after performing sudden quenches in μ from a very small value characteristic of the liquid phase (low density) to a high value corresponding to the glassy phase. Performing a quench in μ is similar to the application of a sudden compression; we raise the density of the system
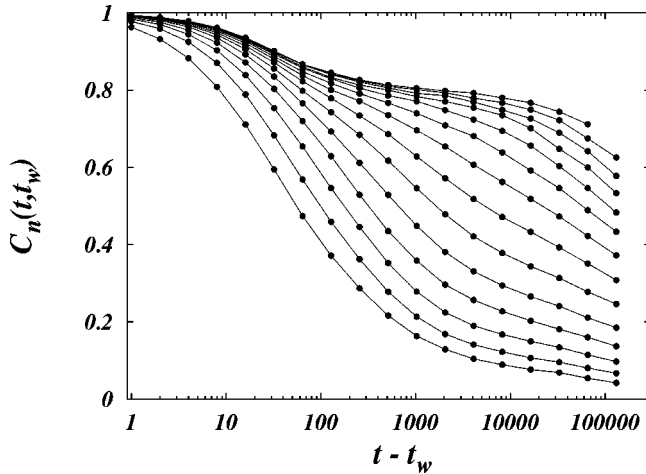
FIG. 1. Density autocorrelations after a quench to $\mu=10$ at $T=1$ and $J=10$ for $L=20$. The waiting times range from 2^5 (bottom) to 2^{17} (top), and the averages are over 50 samples.

FIG. 2. Asymptotic density for different compression rates, ranging from 10^{-2} to 10^{-6} (bottom to top). Inset: power law fitting for several values of μ.

keeping the ratio $\mu/J \lesssim 1$ in order to prevent close packing. Connected two point correlations can be defined as

$$c(t,t_w) = \frac{1}{N} \sum_i n_i(t)n_i(t_w) - \rho(t)\rho(t_w), \qquad (2)$$

where the global density at time t is given by $\rho(t) = N^{-1}\Sigma_i n_i(t)$. We now define the density autocorrelations as $C_n(t,t_w) = c(t,t_w)/c(0,t_w)$.

In Fig. 1 the behavior of $C_n(t,t_w)$ is shown as a function of t in a semilog plot after a quench in chemical potential to a value $\mu=10$, for waiting times between 2^5 and 2^{17}. A typical aging scenario is present, signaling the slowing down of the dynamics as the waiting time grows. For the longest waiting times the correlation presents a rather fast relaxation to a plateau in which the system evolves in quasiequilibrium: the dynamics is stationary, and the fluctuation-dissipation relations hold. The plateau separates two time scales typical of glassy systems: a β (fast) relaxation for short times and an α (slow) relaxation at longer times, corresponding, respectively, to the fast movements of the particles inside the dynamical cages and the large scale, cooperative process that takes much more time in order to rearrange the cages. Moreover, in this very long time regime ($t-t_w \gg t_w$), the system falls out of equilibrium, the correlations decay to zero asymptotically, and time translation invariance no longer holds with the corresponding violation of the fluctuation-dissipation theorem (FDT), as will be shown in the following sections. A good scaling of the correlation functions is obtained assuming a time dependence of the form $h(t_w)/h(t+t_w)$ with $h(x)$ given by $h(x) = \exp[(1-\alpha)^{-1}(x/\tau)^{1-\alpha}]$, where $\alpha<1$, and τ is a microscopic time scale [21]. This form is quite general as one recovers the cases of a simple t/t_w dependence (full aging) when $\alpha=1$, and stationary dynamics when $\alpha=0$ [20]. A similar aging scenario was found, associated with the relaxation of internal degrees of freedom [21].

III. SLOW AND FAST COMPRESSIONS

When the system is gently compressed the glass transition depends on the rate of compression. For a fixed temperature
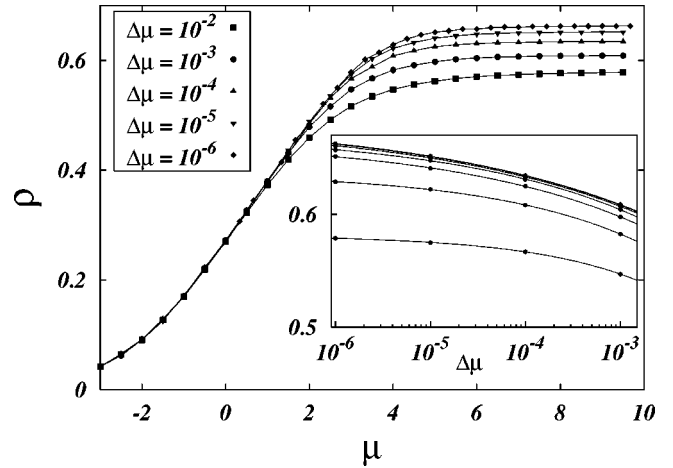
we have done simulations of slow compression experiments, where at each Monte Carlo step μ is increased by a quantity $\Delta\mu$. Figure 2 shows the evolution of the density for several compression rates, ranging from 10^{-2} to 10^{-6}. It can be noted that for slower compressions, the final density is higher. Up to $\mu\approx1$ the density remains small enough, and the system is able to equilibrate sufficiently fast, regardless of $\Delta\mu$, and all curves collapse. As the density increases, the equilibration time also increases since the system cooperative rearrangement involves a larger number of particles in a smaller region. In analogy with cooling experiments, for each compression rate the system falls out of equilibrium at a different value of μ and the asymptotic density increases with decreasing rates. The points where the curves for each rate depart from the master curve define the glass transition point μ_g. The dependence of μ_g on the compression rate is characteristic of glass formers, and is thought to be a consequence of activated processes: no cooling (compression) rate dependence is observed in mean field models where the glass transition appears at a fixed temperature (chemical potential). For a fixed μ, by decreasing the compression rate, the density $\rho(\mu)$ tends to the equilibrium density $\rho_\infty(\mu)$ as a power law $\rho_\infty(\mu) - \rho(\mu) \propto \Delta\mu^{-b}$, as can be seen in the inset of Fig. 2, the parameters depending on the value of μ. The extrapolated equilibrium value is slightly higher than the one obtained upon fast compressions, as will be shown below.

In analogy with temperature cycling experiments in spin glasses, which show the onset of irreversible processes, here, by increasing and decreasing the chemical potential at a given rate, hysteresis cycles can be produced whose internal area increases with $\Delta\mu$. Moreover, the chemical potential range in which the system behaves in an irreversible way also increases with $\Delta\mu$. In Fig. 3 the hysteresis curves are presented for several cycling rates. Note that the lower left part of the cycle coincides with the equilibrium curve, and for very slow rates the cycle tends to disappear, and we recover the above annealing equilibrium curve. As before, the maximum achieved density increases for slower rates.

Instead of slowly compressing the sample, high densities can also be obtained by a fast compression analogous to temperature quenching experiments. Here we consider an
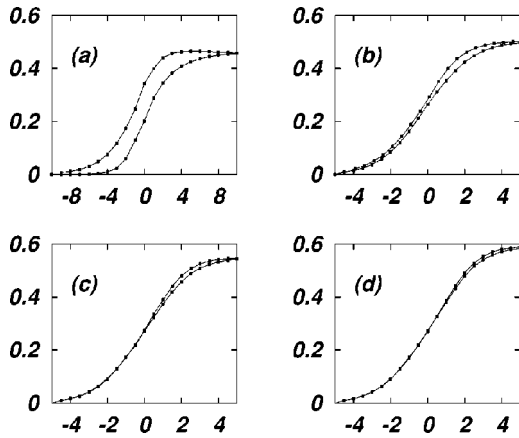
FIG. 3. Hysteresis curves (ρ vs μ) from cycling experiments in a $L=6$ system ($T=1$ and $J=10$). Note the different x-axis scale of (a). The cycling rates are, from (a) to (d), 1, 10^{-1}, 10^{-2}, and 10^{-3}.

initial state with an empty lattice, corresponding to $\mu=-\infty$. Then the chemical potential is suddenly increased to a value above the critical one. In Fig. 4 we show how the density increases after a sudden quench to different μ values, ranging from 1 to 10. For all $\mu<\mu_c\simeq5.5$ the density converges more or less rapidly to an asymptotic value, which depends on μ. For $\mu>\mu_c$ the density increases with a law $\rho(t)$ which seems to be independent of the chemical potential, and that converges to the asymptotic value with a power law: $\rho_\infty-\rho(t)\propto t^{-\alpha}$. The best value for the parameters are $\alpha\simeq0.47$ and $\rho_\infty\simeq0.673$, slightly lower than the value obtained in the slow compressions. In contrast to a sudden compression, by gently annealing the system can approach equilibrium more efficiently. Nevertheless one can expect that the equilibrium density will be reached after a quench in a much longer time scale driven by activated processes. In Fig. 5 we show the relaxation of the density after a sudden compression to $\mu=10$, deep in the glass phase.

If we assume that the density asymptotic value is essentially determined by the amount of frustration present in a sample, then it is possible to calculate the range of allowed values for ρ_∞. In a sample with no frustration, obviously

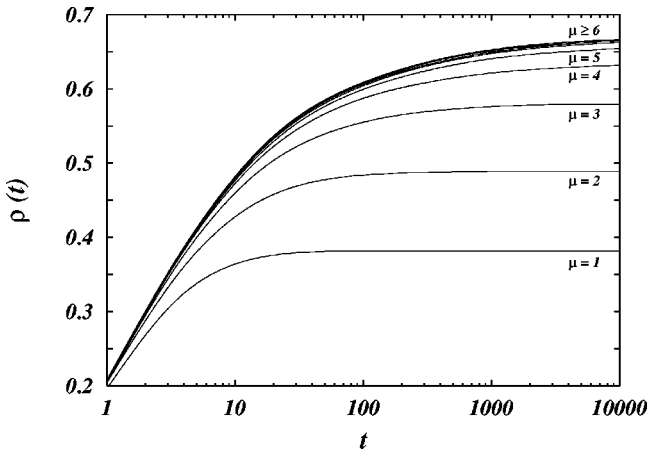FIG. 4. Increasing of the density in a $L=40$ system after a sudden quench in the chemical potential ($T=1$ and $J=10$). All the data for $\mu\geqslant6$ collapse on the same curve, which can be well fitted by a power law (see the text).
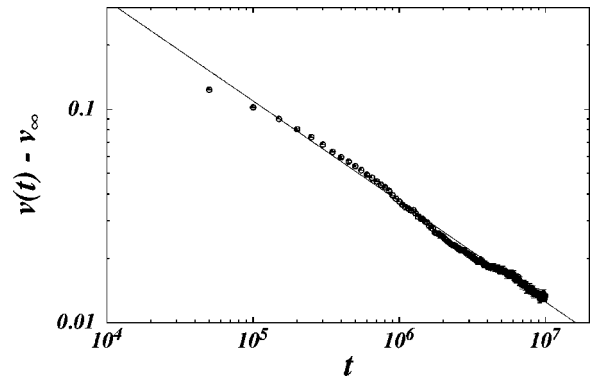

FIG. 5. Decay of the specific volume after a quench to $\mu=10$ for a lattice with $L=6$. The solid line is a power law fit over the last two decades, $v(t)=v_\infty+at^{-\alpha}$, with $\alpha\simeq0.47$ and $v_\infty=1/\rho_\infty\simeq1.48$ ($\rho_\infty\simeq0.673$).

$\rho_\infty^{\max}=1$, while in a fully frustrated sample we have that $\rho_\infty^{\min}=5/8=0.625$. A fully frustrated sample has interactions ε_{ij}, such that every plaquette is frustrated. The value we find for the random model, $\rho_\infty\simeq0.673$, falls in this interval, as it should, and is not very far from the one found in the fully frustrated case. This would suggest that the FILG defined on a fully frustrated lattice may be an interesting nonrandom model with features similar to those presented in this paper. In fact we believe that the glassy behavior of the FILG is based much more on its frustration rather than on its randomness.

As long as activated processes do not enter the scene we would expect a behavior reminiscent of mean field models. In the thermodynamic limit, mean field theory for the p-spin spin glass predicts that the internal energy will relax with a power law to a threshold value E_{th} greater than the equilibrium one [10]. The absence of activated processes will prevent the system from escaping the threshold states, and it will be kept out of equilibrium forever. In a true glass the relaxation of the density at sufficiently low temperatures should behave this way. In the case of the FILG we do not know what the equilibrium density is, so in order to test the previous hypothesis we have measured autocorrelations at constant density.

Considering again the connected two times autocorrelations [Eq. (2)], in Fig. 6 we present results of simulations of quenches at fixed densities. The upper figure shows results for a density that is slightly below the critical one ($\rho=0.67$) for several waiting times t_w. There exists a characteristic waiting time after which all the curves collapse on a master one, meaning that aging is interrupted and time translation invariance (TTI) is recovered. The relaxation preserves the characteristic two steps with equilibrium dynamics for large t_w. On the other hand, for a density $\rho=0.68$, slightly above the critical one, the system seems to age forever, as can be seen in the lower figure. In this case, even for the largest waiting times, the quasiequilibrium regime is followed by an out of equilibrium relaxation where TTI no longer holds and fluctuation-dissipation relations are violated. The behavior in this two cases is qualitatively different, and is reminiscent of mean field behavior with a threshold or critical value for the density. This will be reflected also in the form in which the fluctuation-dissipation theorem
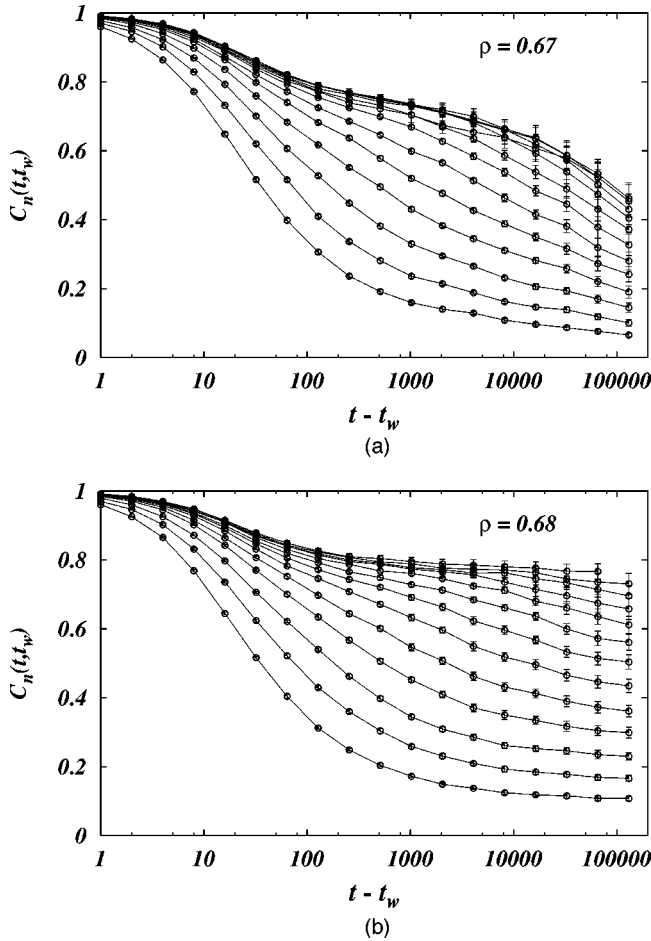
FIG. 6. Decay of the density autocorrelations after a quench at a constant density and $L=20$. Note that for $\rho=0.67$ (top) and moderate waiting times, the dynamics becomes stationary and aging stops, quite different from what happens for $\rho=0.68$ (bottom).

is violated, as will be discussed below.

In real space, one way of seeing aging effects is looking at the diffusion properties of the particles. The averaged mean square displacement in the time interval (t,t_w) is defined by

$$R^2(t,t_w) = \frac{1}{N} \sum_i a_i(t,t_w)[\vec{r}_i(t) - \vec{r}_i(t_w)]^2, \quad (3)$$

where the function $a_i(t,t_w)$ is 1 if the ith particle is present at both times t and t_w, and is 0 otherwise. In this way only particles that do not leave the system enter the measures. Obviously, if the density is kept constant, $a_i=1\,\forall i$. For the smallest waiting times, the density is low and diffusion is like in a simple fluid, R^2 being linear in t (see Fig. 7). Only for large times does the density attain a large value, cages are formed trapping the particles, and the diffusion is arrested, as signaled by the appearance of a plateau. For larger t_w and $t \ll t_w$, the particles "rattle" inside "the cages" formed by their neighbors and the diffusion is still normal, R^2 again being linear in t. The fact that the first linear regime is longer the smaller t_w is simply because for larger t_w the density at $t=0$ is larger. As soon as R^2 is comparable to the cage linear size, the diffusion halts and a plateau is attained. To escape from the cage (hence from the plateau), a large, cooperative rearrangement must occur among neighbor cages. This slow
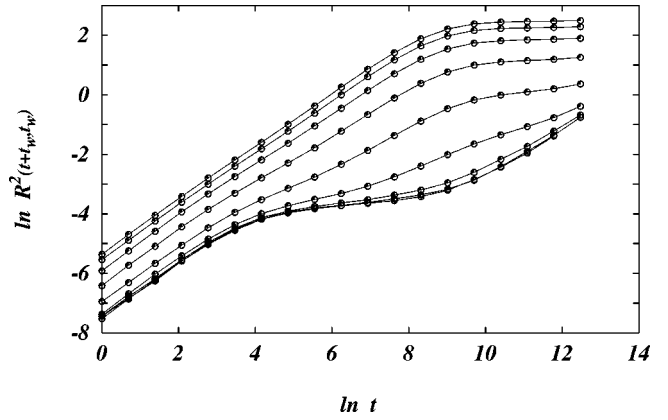

FIG. 7. Two time mean square displacement after a quench for $J=10$, $T=1$, and $L=20$. From top to bottom: smaller to higher t_w.

phenomenon is reflected in the extension of the plateau. Moreover, for larger times we are essentially measuring the diffusion of the cages, which can be seen as the second linear regime present in Fig. 7. From this figure it is clear that aging effects with characteristic dynamical regimes are also present in real space properties of the system.

IV. FDT

When glasses evolve slowly out of equilibrium fluctuation-dissipation relations are no longer valid. Instead, in computer simulations and mean field approximations a generalized relation is obtained [10,20,22],

$$R(t,t_w) = \frac{X[C(t,t_w)]}{T} \frac{\partial C(t,t_w)}{\partial t_w}, \quad (4)$$

where $C(t,t_w)$ is a two times correlation function and $R(t,t_w)$ with $t>t_w$ is the associated response. T is the heat bath temperature and $X(C)$, the fluctuation-dissipation ratio (FDR) is a function that measures the departure from the FDT: at equilibrium $X=1$ and the usual FDT is recovered, while in the out of equilibrium regime, $X<1$. The function X turns out to be a constant in mean field models of glasses, signaling that the asymptotic dynamics of the system is dominated by only one time scale (apart from the FDT scale). In this time scale, corresponding to the aging regime, the slow degrees of freedom are at an effective temperature different from the bath one and that depends on the FDR as $T_{eff}=T/X$ [23]. Recently, the first attempt at an experimental measurement of this effective temperature was made in glycerol glass [24].

In a finite system aging will eventually be interrupted due to activated processes, leading the system to equilibration at the temperature of the bath. Nevertheless, the true role of activated processes in the long time dynamics of glassy systems still remains to be understood. While an analytical approach to the problem is very difficult, one may gain insight from simulations on finite systems.

We have measured the FDR on the FILG [25]. The main result is shown in Fig. 8, where X is given by minus the derivative of the data curves. In this case we measure density correlations and associated compressibilities (for details, see Ref. [25]). This result was obtained in a lattice of linear size
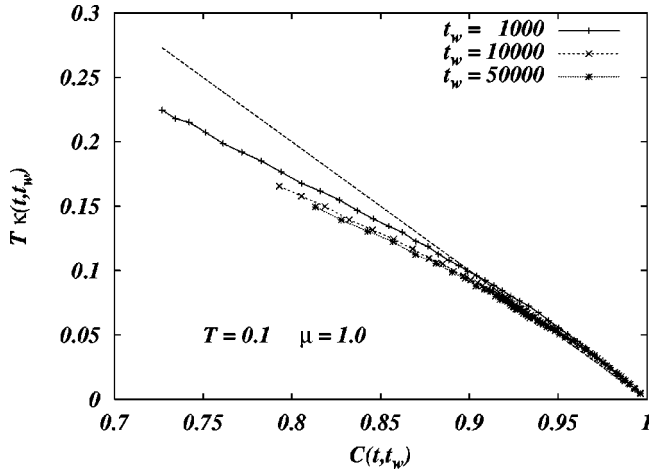
FIG. 8. Integrated response versus density correlations for three waiting times (see the text).

$L = 30$. The result is the one expected for a model having only two dominating time scales: the FDT one, when $C > q_{EA}$; and another one, when the system is relaxing very slowly out of equilibrium and $C < q_{EA}$, q_{EA} being the Edwards-Anderson (EA) order parameter [6]. The constancy of X in the aging regime is exactly what is predicted by mean field theory.

What is very remarkable is that this constancy seems to be valid not only for the asymptotic curve ($t_w \rightarrow \infty$), but also for finite (although large) t_w curves. Then we can express the FDR as a function only of the smaller time, t_w, and we observe that it changes very slowly with t_w.

We also note that the fact that X seems to depend only on the smaller time is in agreement with some recent analytical results. In Ref. [26] it was shown that slow glassy dynamics can be viewed as an evolution between "quasistates," where the system (almost) equilibrates before relaxing further. When the field is switched on at time t_w it will select a particular set of quasistates, those with the "right" magnetization. If this is the case then the externally induced small perturbation [27] will regress in the same way a spontaneous fluctuation does, and one can show [28] that the FDR may depend on the smaller time, but not on the larger one. And this is exactly what we have observed numerically in the FILG model.

Nevertheless, in contrast with mean field predictions, the curves for different temperatures and chemical potentials in the glass phase (for a fixed large t_w) remain parallel, simply shifting upward with a corresponding decrease in the value of the EA parameter [25]. This is reasonable as one expects that the FDT regime will be the only one present as $T \rightarrow T_g$. This behavior is not observed in mean field approximation, where the EA parameter has a discontinuous jump at T_g, and X changes continuously for $T < T_g$. Other studies in long range models seem to point out a continuous approach of T_{eff} to the bath one [29]. A systematic study of these effects is necessary in order to understand the underlying mechanisms responsible for them.

It is not clear whether the system will also undergo a static transition with one step of replica symmetry breaking, as the off-equilibrium dynamics would suggest. Thermalization at $T \lesssim T_g$ is very hard to attain, and so we did not suc-
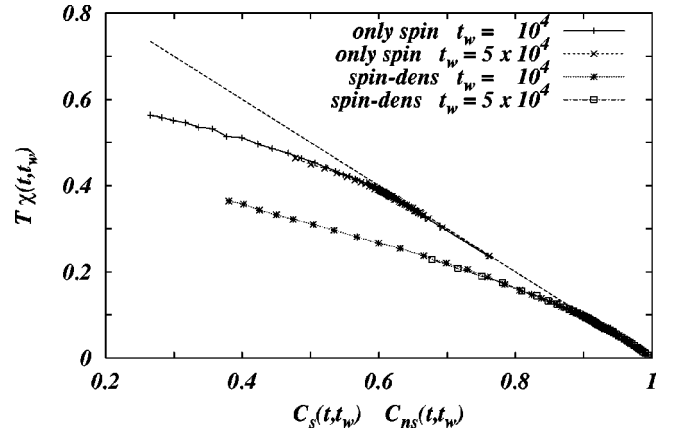

FIG. 9. Integrated response vs spin correlations (see text).

ceed in answering this question. However, even in the case that all the observed dynamical features would not correspond to an underlying static transition, and would eventually disappear as the system equilibrates, the results are interesting for at least two reasons. First, real glassy systems can be in the off-equilibrium regime all along their life, and so a study of their out of equilibrium behavior rather than the static behavior is more relevant. Second, even if what we are observing is due to finite time effects (although very large), it is very remarkable that it is well described by mean field approximations. Maybe it is the case that, on time scales where activated processes are very rare, mean field theories (that completely neglect activated processes) are a good approximation.

We have also measured the FDR associated with the relaxation of the spin or internal degrees of freedom. One can consider the spin-spin autocorrelation

$$C_s(t,t_w) = \frac{1}{N} \sum_i S_i(t) S_i(t_w), \qquad (5)$$

or, taking spins only from occupied sites, the spin-density-spin-density auto correlation

$$C_{ns}(t,t_w) = \frac{1}{N} \sum_i S_i(t) n_i(t) S_i(t_w) n_i(t_w). \qquad (6)$$

By applying suitable perturbations, like small random magnetic fields, in the standard way one can define integrated responses corresponding to the correlations defined above. The parametric plot of the integrated responses versus correlations is shown in Fig. 9.

The interesting result which shows up here is that, qualitatively, the FDR is the same in all three cases. Furthermore, fits to the data show approximately the same asymptotic value of X. While the data for spin-density-spin-density and density-density variables are exactly on the same straight curve, the data for spin-spin variables depart from the FDT line at a smaller value of the Edwards-Anderson parameter. This is due to the fraction of spins placed on empty sites.

The fact that we have measured the same effective temperature T_{eff} perturbing different degrees of freedom is remarkable. It is known that when different degrees of freedom are coupled they must reach the same temperature. However,
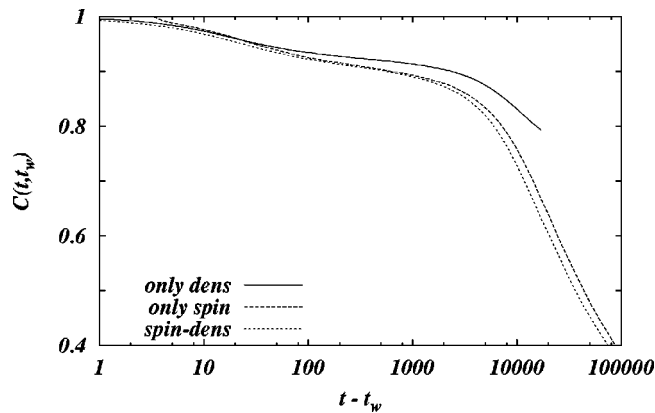
FIG. 10. Several possible correlations C_{ns}, C_s, and C_n for $t_w = 10^4$.

to our knowledge this is the first time that such behavior has been measured in the aging regime of a finite-dimensional system.

It is worth noting that there is strong evidence [15] that internal degrees of freedom are responsible for a thermodynamic spin glass transition at a temperature near T_g, the structural glass transition temperature. The constant value of the FDR for the spin variables indicates that the transition should be typical of systems with one replica symmetry breaking. If this is confirmed we have at hand a finite model, with short range interactions, which presents a discontinuous transition, like that present in mean field models as the p-spin model. In fact, at a mean field level, a line of discontinuous transitions has been found in models closely related to the FILG [18]. More work is needed in order to test this possibility in the short range model.

For the sake of comparison, in Fig. 10 results for all three correlations studied are shown for $t_w = 10^4$. Note that the correlation involving both occupation and spin variables is always smaller than the other two: $C_{ns} < \min(C_n, C_s)$. For small times, C_{ns} is dominated by the particle dynamics, and for large times by the internal degrees of freedom dynamics.

V. CONCLUSIONS

We have described the main characteristics of the out of equilibrium dynamics of the three-dimensional frustrated Ising lattice gas. This shows a very complex and interesting phenomenology similar to that observed in real glass formers. The glass transition seems to have a purely dynamical origin, as no evidence of singular behavior was found either in the linear or nonlinear compressibilities. Aging dynamics is present in both density and internal degrees of freedom, and the decay of autocorrelations is similar to that observed in molecular dynamics simulations of Lennard-Jones glasses. Cage effects are evident both in density relaxation and on diffusion properties where a clear characterization of different regimes is possible. From slow compression experiments different densities are reached depending on the compression rate, and hysteresis is observed from cycling experiments. After a sudden compression the density slowly approaches a limiting value. Aging experiments at fixed densities slightly above and below this limiting value show clear qualitative differences, showing that this density may separate two different dynamical regimes.

The overall scenario is very reminiscent of mean field scenarios for the glass transition, except for the presence of a compression rate dependence which is absent in mean field. Interestingly, the form of the fluctuation-dissipation theorem violations is exactly that predicted in mean field approximations, i.e., a constant fluctuation-dissipation ratio . This means that this model presents two very separated time scales. The effective temperature in the out of equilibrium scale is nearly temperature independent in the glassy phase. This raises the question of whether or not activated processes play an important role in its dynamics. The same constant effective temperature is observed as associated with the internal degrees of freedom. At the mean field level, a constant effective temperature has been obtained in systems characterized by one step replica symmetry braking (1RSB). Thermodynamically, a phase transition with a divergent susceptibility associated with internal degrees of freedom is observed. This may be the first realization of a glassy phase characterized by 1RSB in a finite-dimensional model. The presence of a static transition associated with density variables at a low "Kauzmann temperature" $T_K < T_g$ remains an open problem in this model. It would be interesting to study in more detail how the restoration of FDT relations is achieved as T_g is approached from below in order to test the strength of the time scale separation. Also, activated processes may show up for bath temperatures larger than those explored in these simulations as long as frustration begins to be lifted by thermal activation.

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