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2002 J. Phys.: Condens. Matter 14 1549

(http://iopscience.iop.org/0953-8984/14/7/312)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 1549–1556 PII: S0953-8984(02)31460-7

From an unconstrained model with quenched interactions to a constrained model with annealed interactions

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Received 3 December 2001
Published 7 February 2002
Online at stacks.iop.org/JPhysCM/14/1549

Abstract

The frustrated lattice gas model is studied in the quenched version where the interactions are quenched random variables, and in the annealed version where the interactions are allowed to evolve in time with a suitable kinetic constraint. The dynamical nonlinear susceptibility, recently introduced by Donati *et al*, is evaluated. In the annealed version we observe a behaviour very similar to the results for the p-spin models in mean field, and those for a Lennard-Jones mixture as found by Donati *et al*. In the quenched version we observe a substantially different behaviour of the dynamical susceptibility. The results suggest that the behaviour of the dynamical susceptibility in the annealed model can be interpreted as the imprint of the thermodynamic transition present in the quenched model and signalled by the divergence of the static nonlinear susceptibility. A similar mechanism might also be present in glassy systems.

1. Introduction

The frustrated lattice gas model has been recently introduced in the context of the glass transition [1].

In the quenched case the model is a spin glass diluted with lattice gas variables; being made up of diffusing particles, it is suitable for studying 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 [2] properties closely related to those of p-spin models. In three dimensions (3D), at low enough temperatures, numerical simulations [3] show a behaviour of the diffusion coefficient very similar to that experimentally observed in fragile liquids [4]. 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 also observed in spin glasses, but it is absent in glassy systems, where there is no sharp thermodynamic transition characterized by the divergence of a thermodynamical quantity analogous to the nonlinear susceptibility.

We have also studied the model in the annealed version [5], where the interactions are allowed to evolve with a kinetic constraint. We find that the dynamical behaviour fits quite well the predictions of the mode coupling theory for supercooled liquids [6]. It is also easy to show that the model does not exhibit any thermodynamic transition; consequently there is no divergence in the nonlinear susceptibility.

Recently Donati *et al* [7] have introduced a dynamical nonlinear susceptibility both for spin models and for structural glasses. They have shown that in the mean field p-spin spherical models [8] (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

$$H = \sum_{i_1<\cdots<i_p} J_{i_1\cdots i_p} S_{i_1} \cdots S_{i_p} \tag{1}$$

where $p \geqslant 3$, the couplings $J_{i_1\cdots i_p}$ 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

$$\chi(t) = \beta N(\langle q(t)^2\rangle - \langle q(t)\rangle^2) \tag{2}$$

where $q(t) = \frac{1}{N}\sum_i S_i(t')S_i(t'+t)$ is the overlap between the states at times t' and $t'+t$. Solving the equation of motion for $\chi(t)$ at a temperature higher than T_D, Donati *et al* 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 behaviour has also been found in molecular dynamics simulation performed for a Lennard-Jones mixture.

We have evaluated $\chi(t)$ in the frustrated lattice gas model, in both the quenched and the annealed version. Whereas in the quenched case $\chi(t)$ shows a behaviour substantially different from that obtained in glass forming systems, in the annealed case it exhibits a maximum with a behaviour similar to that found in the mean field p-spin models and in molecular dynamics simulations of a Lennard-Jones mixture.

2. The frustrated lattice gas model

2.1. The quenched model

Recently a lattice model, which has mean field properties closely related to those of p-spin models, has been introduced [1] in connection with the glass transition. This model is a diluted spin glass which, since it comprises diffusing particles, is well suited for the study of quantities that are usually important in the study of liquids, such as the diffusion coefficient or the density autocorrelation functions. The Hamiltonian of the model is

$$-\beta H = J\sum_{\langle ij\rangle}(\epsilon_{ij}S_iS_j - 1)n_in_j + \mu\sum_i n_i \tag{3}$$

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

This model reproduces the Ising spin glass in the limit $\mu \to \infty$ (all sites occupied, $n_i \equiv 1$). In the other limit, $J \to \infty$, the model describes a frustrated lattice gas with properties recalling

those of a 'frustrated' liquid. In fact, the first term of the Hamiltonian (3) implies that two nearest-neighbour 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 non-symmetric shape. Two particles can be nearest neighbours only if their 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 as in the spin glass model and correspond in the liquid to those loops which, due to geometrical hindrance, cannot be fully occupied by the particles.

In the case $J = \infty$ the model has a maximum density $\rho_{\max} \simeq 0.68$. It has been shown that there exists some density $\rho_c \simeq 0.62$ where the system has a transition of the type of 3D p-spin models [9], with a divergence of the static nonlinear susceptibility

$$\chi_{\mathrm{SG}} = \frac{1}{N} \sum_{ij} [\langle S_i n_i S_j n_j \rangle^2] \tag{4}$$

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

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

$$q(t) = \frac{1}{N} \sum_i S_i(t') n_i(t') S_i(t'+t) n_i(t'+t) \tag{5}$$

and for the dynamical susceptibility

$$\chi(t) = N[\langle q(t)^2 \rangle - \langle q(t) \rangle^2] \tag{6}$$

where the average $\langle \cdots \rangle$ is done on the reference time t'. In figure 1 we show 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 by averaging over a time interval for t' of 6×10^6–8×10^7 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. In figure 2 we show the dynamical susceptibility $\chi(t)$ for the same size and values of the density as in figure 1. Note that $\chi(t)$ grows monotonically and has no maximum at finite time. The asymptotic value $\chi(\infty)$ corresponds to the static susceptibility (4), and therefore has a divergence at the density $\rho_c \simeq 0.62$.

2.2. The annealed model

We have studied the frustrated lattice gas model (3) in the case where the interactions $\epsilon_{ij} = \pm 1$ are annealed. When we evaluate the partition function of the model, we must consider in this case not only the S_i and n_i but also the ϵ_{ij} as dynamical variables. Thus, summing over the ϵ_{ij} and S_i we obtain, apart from an irrelevant factor, $Z = \sum_{\{n_i, S_i, \epsilon_{ij}\}} \mathrm{e}^{-\beta H} = \sum_{\{n_i\}} \mathrm{e}^{-\beta H_{\mathrm{eff}}}$, where

$$-\beta H_{\mathrm{eff}} = -K \sum_{\langle ij \rangle} n_i n_j + \mu \sum_i n_i \tag{7}$$

and $K = -\ln(1 + \mathrm{e}^{-2J}/2)$. Therefore the static properties of the model are equal to those of a lattice gas with a repulsion between nearest-neighbour 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 $T_{\mathrm{eff}} = 4\ \mathrm{K}^{-1}$, which is always greater than the critical temperature of the 3D antiferromagnetic Ising model $T_c \simeq 4.5$. Therefore we can conclude

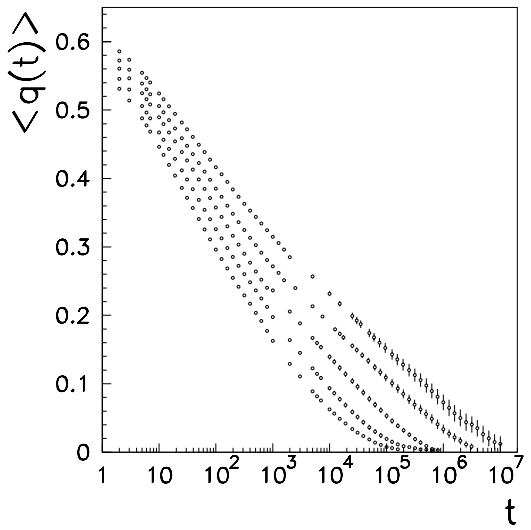

Figure 1. Relaxation functions of the self-overlap in the quenched model, for a system of size 16^3 and densities $\rho = 0.58, 0.59, 0.60, 0.61, 0.62$ (density increasing from bottom to top).

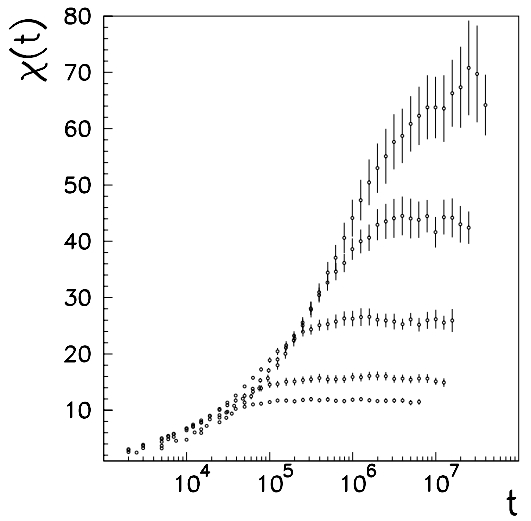

Figure 2. Dynamical susceptibility in the quenched model, for a system of size 16^3 and densities $\rho = 0.58, 0.59, 0.60, 0.61, 0.62$ (density increasing from bottom to top).

that the model (7), and also then the model (3) with annealed interactions, does not exhibit any thermodynamic transition. In the following we always consider the model with $J = \infty$.

We assume a dynamics for the variables ϵ_{ij} with a kinetic constraint, namely ϵ_{ij} can change its state only if the sites i and j, and all their nearest neighbours, are empty; in this way the states accessible to a given particle can 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 if they were frozen, playing the role of 'self-induced quenched' variables.

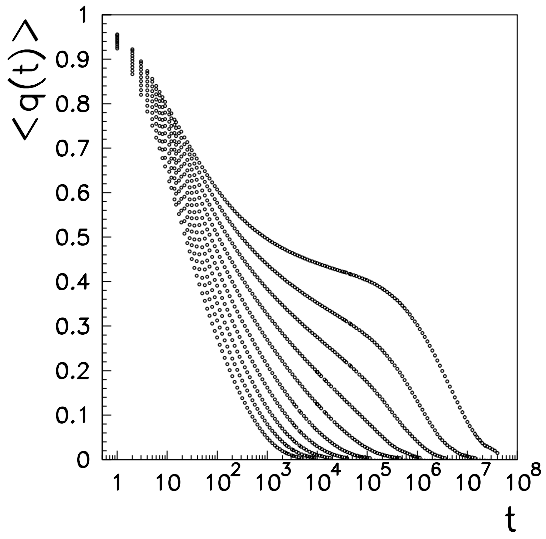

Figure 3. Relaxation functions of the self-overlap in the annealed model, for a system of size 16^3 and densities $\rho = 0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.60, 0.61$ (density increasing from bottom to top).

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

(1) one starts from an equilibrium configuration obtained at some density ρ;
(2) at each step of dynamics an interaction ϵ_{ij} is randomly chosen and is changed if the sites i and j, and all their nearest neighbours, 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-neighbour 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 neighbours of the destination site must satisfy the interaction with the spin of the chosen particle. If the particle cannot move to the chosen site the move is rejected;
(5) the clock advances one unit of time.

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

In figure 3 we show the relaxation functions of the self-overlap (5), for a system of size 16^3, for various densities between $\rho = 0.52$ and 0.61. Each curve is obtained by averaging over a time interval for t' of 3×10^6 to 10^8 Monte Carlo steps. Observe that, for high density, the relaxation functions clearly develop a two-step relaxation, signalling the existence of two well separated time scales in the system. We interpret the initial short time decay of the relaxation functions as due to the motion of the particles in the frozen environment, which on this time scale appears as quenched, while the second decay is due to the evolution of the environment,

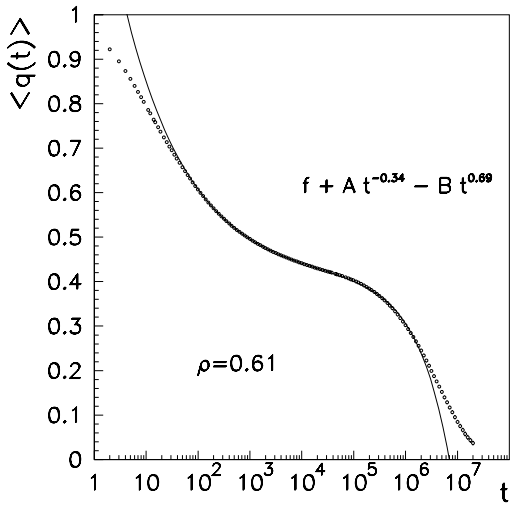

Figure 4. Fit of the intermediate time part of the relaxation function of the self-overlap, for density $\rho = 0.61$, with the fitting function $f + At^{-a} - Bt^{b}$, where the fitting parameters are f, A, B and λ, and a and b are given by the relation (9).

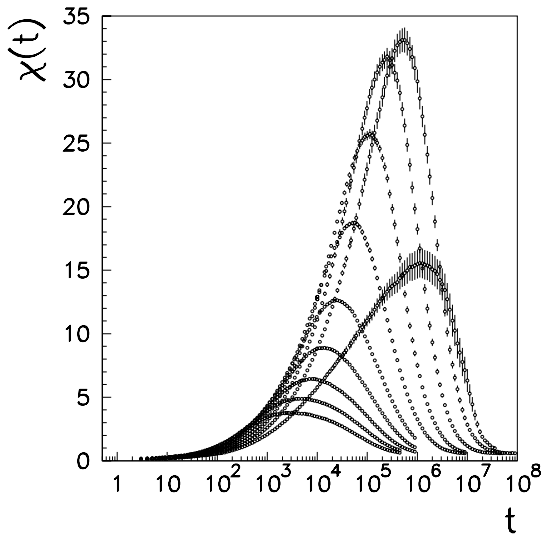

Figure 5. Dynamical susceptibility in the annealed model, for a system of size 16^3 and densities $\rho = 0.52, 0.53, 0.54, 0.55, 0.56, 0.57, 0.58, 0.59, 0.60, 0.61$ (density increasing from left to right).

and the final relaxation to equilibrium of the system. We tried to fit the intermediate time part, corresponding to the plateau, of the relaxation function of the overlap for density $\rho = 0.61$, with the function predicted by the mode coupling theory [6] (in a simplified form):

$$\langle q(t) \rangle = f + At^{-a} - Bt^{b} \tag{8}$$

where a and b are given by the relation

$$\frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)} = \lambda \tag{9}$$

and f, A, B and λ are the fitting parameters. The result is shown in figure 4, where the full curve is the fitting curve with $a = 0.339 \pm 0.002$ and $b = 0.69 \pm 0.01$.

In figure 5 we show the dynamical nonlinear susceptibility (6) for the same system size and values of the density as in figure 3. It has the same behaviour as the p-spin model in mean field and as the molecular dynamics simulations of the Lennard-Jones binary mixture, namely a maximum $\chi(t^*)$ that seems to diverge, together with the time of the maximum t^*, as the density increases. For the highest density, the maximum of $\chi(t)$ decreases, possibly due to finite size effects, too short an observation time, or a change in the dynamics above some critical density. This fact is observed also in molecular dynamics simulations of Lennard-Jones liquids [10]. We find that the maximum $\chi(t^*)$ as a function of the density can be fitted quite well (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 $\chi(\infty) = \rho^2$.

3. Conclusions

The frustrated lattice gas model in the quenched version has a thermodynamic transition at a critical density, where the static nonlinear susceptibility diverges. The annealed model, which does not exhibit any thermodynamic transition, consequently does not show any critical behaviour of the static susceptibility; on the other hand, we observe a critical behaviour of the dynamical susceptibility similar to that observed in glass forming systems.

We conclude that the thermodynamic transition, present in the quenched model and signalled by the divergence of the static susceptibility, manifests itself in the annealed model in the critical behaviour of the dynamical susceptibility. This behaviour seems a consequence of the fact that, for sufficiently short times, the interactions can be considered as quenched variables. Since the annealed model shows a behaviour reminiscent of supercooled glass forming liquids [5], the results suggest that also in glass forming liquids the behaviour of the time-dependent nonlinear susceptibility may be due to the presence of slow degrees of freedom which act as quenched variables on short time scales. 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 interaction; in our case the statics of the model is instead described by a trivial Hamiltonian, while the complex dynamics is due to the kinetic constraint.

Acknowledgments

This work was partially supported by the European TMR Network-Fractals under contract no FMRXCT980183 and from INFMPRA(HOP). We acknowledge the allocation of computer resources from INFM Progetto Calcolo Parallelo.

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