Kob-Andersen model: A nonstandard mechanism for the glassy transition

S. Franz,[1] R. Mulet,[1,*] and G. Parisi[2]
[1]*The Abdus Salam Centre for Theoretical Physics, Condensed Matter Group, Strada Costiera 11, P.O. Box 586, I-34100, Trieste, Italy*
[2]*Dipartimento di Fisica, SMC and UdR1 of INFM, INFN, Università di Roma "La Sapienza," P. A. Moro 2, 00185 Rome, Italy*
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We present results reflecting the analogies between the Kob-Andersen model and other glassy systems. Studying the stability of the blocked configurations above and below the transition we also give arguments that support their relevance for the glassy behavior of the model. However, we find, surprisingly, that the organization of the phase space of the system is different from the well known organization of other mean field spin glasses and structural glasses.

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I. INTRODUCTION

In the last two decades our understanding of the glass transition in spin systems has provided a coherent picture of glassy phenomena at the mean field level [1]. These systems provide the simplest example of systems where complex energy landscapes, with many local energy stationary points, lead to vitrification and to the absence of thermalization over large time scales. At a mean field level, there are spin glass models which show a dynamic transition very well differentiated from the static one. Below the dynamical transition temperature the system is unable to thermalize and get stacked at energies above the equilibrium one. At the same value of the temperature the space of equilibrium states gets disconnected.

The situation is different for real materials, where the sharp transition is not present, and seems to be substituted by a smooth crossover to a dynamics dominated by activated processes [2]. Progress in the last decade of research, however, indicates that many of the aspects of the picture of the glass transition gained from the study of mean field models may well apply to real materials. In fact, while already Kirkpatrick and Thirumalai [3] and Mezard and Parisi [4] noticed the similarity between the thermodynamic transition in structural glasses and spin glasses, later there were found discontinuous transitions in spin glasses without quenched disorder, giving confidence that this analogy was not fortuitous [5,6]. Now, it has been recognized that at least in some approximation, classical first principle models have a phenomenology which resembles that already found in mean field spin glasses [1,7,8].

Moreover, an important feature of the phenomenology of glass forming liquids is the formation of dynamical heterogeneities, characterized by a spatial extension and a given lifetime, both of which increase as the temperature is decreased. These heterogeneities have been found in numerical simulations of various realistic models [9,10] as well as in experiments on colloidal glasses [11], and seem to be a salient feature of landscape dominated glassy systems. In order to quantify the presence of dynamic heterogeneity, it has been proposed to the study four-point density dynamic correlation function. For this quantity mean field theory predicts a peculiar time/temperature dependence, in agreement with the one observed in numerical simulations [12].

A related problem is the physics of granular systems. Since, in general, these systems involve many particles, it is tempting to treat them using the methods of statistical mechanics and, in fact, this approach has become an active field of research for people with a background in this field [13]. Particularly interesting have been the experimental results of the Chicago group who showed that a granular system subject to continuous tapping develops a glasslike transition [14].

An alternative view of the glass transition comes from kinetic models, which have been useful to prove that complex energy landscapes are not a necessary ingredient to have glassy phenomena. Vitrification has been found in simple lattice cellular automata models with kinetic constraints.

An interesting model belonging to this class is the Kob-Anderson model [15], which has been shown by several studies to undergo a structural arrest at densities larger than the threshold one. The phenomenology of the model has been compared with qualitative agreement with the mode coupling theory [2], which proposes an intrinsically kinetic view of the glass transition.

Despite the fact that the mechanisms leading to structural arrest in the model cannot be related to a nontrivial energy landscape, many aspects of the physics of the model are very similar to the phenomenology of mean field glassy systems. In particular, the blockage to the threshold density found in aging experiments in Refs. [16,17] closely resembles the blockage of the internal energy in the dynamics of mean field spin glasses. In addition, it has been recently shown that during aging dynamics, the system probes portions of phase space close to generic random blocked configurations [18], again, in a way reminiscent of mean field glassy phenomenology.

It is tempting in such situations to invoke some universal mechanism underlying structural arrest both in landscape dominated systems, and in kinetically constrained ones. In this paper we investigate the limits to which these analogies can be pushed and to what extent the mechanisms are really universal.

The Kob-Andersen (KA) model, which first emerged as a model to describe the dynamic transition in structural

*Permanent address: Supercond. Laboratory, Fac. Física–IMRE, University of Havana, CP 10400, La Habana, Cuba.

glasses, has also been recently used as a simple model for the jamming transition in granular systems [19,16,18]. While many other lattice models have been proposed to study similar problems [20,21], this one has the advantage of a trivial equilibrium state that can be easily characterized analytically without further assumptions, and that therefore allows a clear comparison between the static and the dynamic properties of the system.

A first test to which we submit the KA model is the computation of the dynamical susceptibility associated to a four-point function, and show that it behaves as expected from mean field theory.

A second point that we investigate is the nature of the blocked states. A lot of emphasis has been recently put on the role of stationary points of the energy surface in glassy dynamics, and the ideal mode coupling transition has been associated with the point where the number of negative directions of the inherent saddles vanishes [22,7].

In other words, while above the mode coupling (MC) point the dynamics spends a lot of time close to saddles, below it spends its time close to minima. The work of Ref. [18] has emphasized the role of the blocked states during aging in the KA model. In this paper we show that while these states are responsible for the glasslike properties of the model, their geometrical organization differs from the organization of the states found in spin and structural glass models.

The remainder of the paper is organized as follows: In Sec. II we define the model and discuss the current understanding in the literature. In Sec. III we present our numerical simulations and discuss the results. Finally in Sec. IV the conclusions are outlined.

II. MODEL

The Kob-Andersen model is a lattice gas defined in a three dimensional lattice of size L^3 where N particles interact by hard core repulsion (i.e., only one particle can be in a site at a given moment) and that evolves using dynamic rules (described below) which are symmetric in time, so that the detailed balance is satisfied.

We first choose a particle at random, then the particle moves if the following conditions are satisfied:

(i) the neighboring site is empty;

(ii) the particle has less than four nearest neighbors;

(iii) the particle will have less than four nearest neighbors after it has moved.

Already in the first paper devoted to the model it was shown that the dynamics becomes slower when the density ρ in the system increases. In particular, the diffusion coefficient vanishes as a power law at the critical density $\rho_c \approx 0.88$ independently of the system size ruling out the possibility that this phenomenon could be associated with the formation of an infinite backbone in the system [15].

More recently, the system has been studied in the presence of a chemical potential [18]. Despite the trivial equilibrium properties of the system, it was proved in a series of papers that below a certain critical density ($\rho_c \approx 0.88$) the system is not ergodic, independently of the chemical potential the density gets blocked at a density lower that the critical density. This density depends on the ''cooling rate.'' Detailed linear response numerical experiments have shown the emergence of an effective temperature. This effective temperature coincides very well with the ''Edwards'' temperature, which can be computed from a uniform measure over blocked configurations. The spatial correlation function obtained by a slow annealing close to ρ_c is very similar to the one expected from the Edwards measure.

While these results and others presented below closely resemble the macroscopic behavior of many glassy systems, we will prove that this analogy can hardly be extended to the organization of the phase space of the system and therefore suggests a nonuniversality of the glassy mechanism.

III. RESULTS AND DISCUSSION

A. Nonlinear susceptibility

It has been recently stressed that glassy dynamics has an inhomogeneous character. There one observes regions of correlated motions whose sizes depend on a control parameter, and that survive for a characteristic time also parameter dependent [12]. This character can be revealed studying the four-point density correlation function. In lattice gas models this can be defined as

$$\chi(t) = N[\langle q^2(t)\rangle - \langle q(t)\rangle^2], \tag{1}$$

where

$$q(t) = \frac{1}{N\rho(1-\rho)} \sum_i [n_i(t) n_i(0) - \rho^2] \tag{2}$$

and the average is performed with respect to different samples. In Ref. [23], based on the theory of disordered systems, it was proposed that in the deep supercooled phase, due to the inhomogeneous character of the dynamics, $\chi(t)$ should display a maximum as a function of time. This maximum appears more and more pronounced, and displaced to larger and larger times as the temperature is decreased (which is equivalent in the KA model to increase the density of particles in the system).

This behavior reflects the geometrical structure of the phase space visited during the evolution of the system and the physics of time scale separation. Along its evolution the system remains blocked in regions of phase space that have longer and longer lifetime, and with more and more correlated density fluctuations as the density is increased. These regions lie close to saddle points of the energy surface, which have lower and lower numbers of escaping directions, until at the dynamical transition the number of negative directions tends to zero.

We have investigated the behavior of the function $\chi(t)$ as a function of the density in the KA model, simulating systems with size $L=10$ and $L=20$, and averaging over 100 samples obtaining errors lower than the 5%. In Fig. 1 we show the behavior of the nonlinear susceptibility as a function of time for various values of the density, showing that qualitatively this function behaves in the same way found in

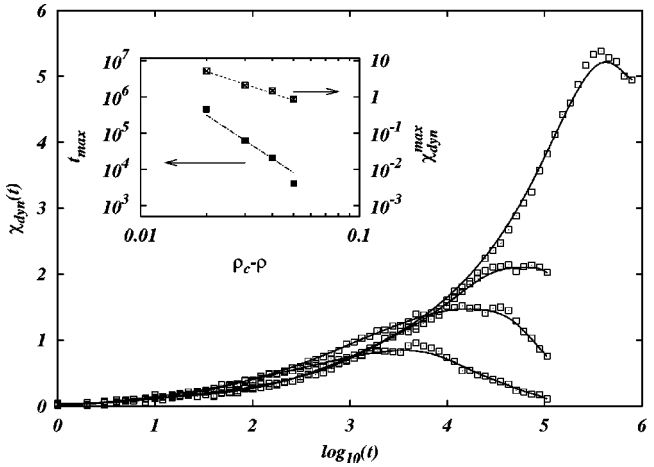

FIG. 1. The nonlinear susceptibility in the KA model as a function of time for different densities. From top to bottom $\rho=0.86$, 0.85,0.84,0.83. The inset shows t_{max} and χ^{max}_{dyn} close to the transition; the lines are power laws (guide to the eyes) with exponents 4 and 2 for t_{max} and χ^{max}_{dyn}, respectively.

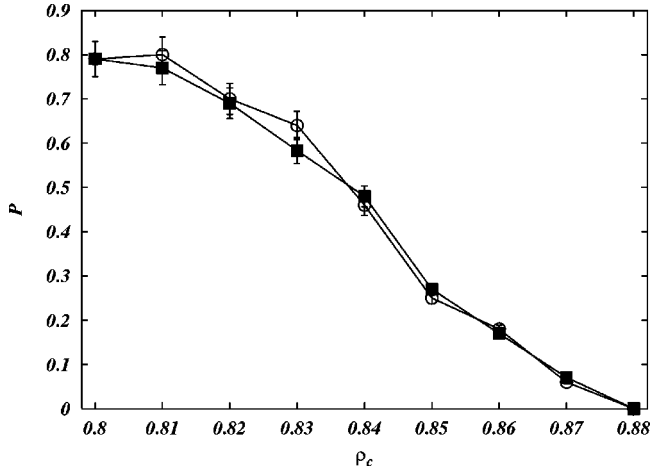

FIG. 2. The unblocking probability as a function of the density. ○, data from the blocked configurations obtained with the auxiliary model; ■, data from block configurations obtained taking a random configuration.

simulations of liquids and in spin models [24] and theorized in Ref. [23]. The maximum, as well as the position of the maximum seem to diverge at the dynamical critical density as power laws with exponents 4 and 2, respectively.

It is interesting to note that in the low density phase, although the KA probes the configuration space ergodically, the dynamics develops correlations which are similar to the ones seen in structural glasses. Even if the infinity time limit of the susceptibility is trivial, due to the fact that the system visits the space ergodically, the dynamics is highly correlated.

In Ref. [18] it was emphasized that during the aging, where dynamics becomes slower and slower, the average value of many quantities approaches the one that can be computed from a measure which is uniform on the blocked configurations and zero otherwise. This was called the Edwards measure, in reference to the analogous concept in granular physics [25]. It remains to be explained why in the aging experiments the system blocks exactly at the value of the density where the fixed density experiments are not ergodic.

B. Stability of the blocked states

In order to understand the role of the blocked configurations at different densities, we studied the stability of the blocked states with respect to the move of a single particle, in a way analogous to the local stability analysis in a complex energy landscape.

To generate blocked configurations with uniform weight, we used the ''trick'' of the auxiliary model introduced in Ref. [18]. There, one associates with each configuration of the lattice gas an energy equal to the number of particles which are free to move according to the KA dynamics. The thermodynamics of this auxiliary model is studied with the help of an an auxiliary temperature $T_{aux}=1/\beta_{aux}$. The Edwards measure can be obtained as the limit $T_{aux}\to 0$ of the Boltzmann measure of the auxiliary model, and can be studied numerically using a simulated annealing procedure where T_{aux} is slowly decreased to zero. This was achieved through standard Metropolis algorithm where the elementary trial moves were random displacements of the particles in the lattice.

In this way, for example, one can compute the Edwards entropy as a function of the density from the thermodynamic integration of the internal energy:

$$S(\rho)=H(\rho)+\int_0^\infty d\beta_{aux}\beta_{aux}U_{aux}(\beta_{aux}), \qquad (3)$$

where $H(\rho)=-\rho\ln(\rho)-(1-\rho)\ln(1-\rho)$ is the entropy of the auxiliary model at $\beta_{aux}=0$.

Once we generated the blocked configurations at different densities with the procedure we explained, we picked a particle at random and moved it to an arbitrary site, and let the system evolve according to the ordinary KA dynamics. The perturbation to the blocked state causes some particles to become free to move, so we detected the number of particles that as a consequence of the perturbations move at least once. We observed two kinds of events: either the displacement of a particle has little effect, and only a small number of particles unblock; or the displacement of the particle completely unblocks the system which starts to move ergodically, after a time which depends on the particle density.

In Fig. 2 we display the estimated unblocking probability, obtained generating 1000 blocked configurations using the simulated annealing as described above and checking how many unblock, as a function of the density (white circles in Fig. 2). At low density, this probability is different than zero in the low density phase which means that even if the system approaches by chance a blocked state, it will always depart from it. The value of the density at which the unblocking probability vanishes is compatible with the critical density $\rho_c=0.88$ of the dynamical instability.

We have also checked that configurations generated with a quench of the auxiliary model form $T_{aux}=\infty$ to $T_{aux}=0$

give rise to the same unblocking probability, hinting that *all* blocked configurations, whether or not measured with uniform probability, have the same stability properties.

C. Geometrical structure of the blocked states

As we have seen, the blocked states are unstable for densities below threshold, while they are stable above threshold. One can ask if this stability property of the blocked states is in correspondence with their geometrical organization in space as it happens in mean field spin glasses [26]. There the stationary points of the energy are saddles above threshold and minima below. It has been shown that the minima are disjointed below threshold: the maximal overlap between minima q_0 is smaller than 1, and tends to 1 as the energy tends to the threshold energy from below, meaning that at that value of the energy one finds minima arbitrarily close to a given minimum. Above the threshold, there is no gap between saddles, and indeed one can show that the logarithm of the number of saddles at overlap q from a given saddle grows as $\Sigma(E,q) \approx N(1-q)$. The threshold energy appears as a kind of percolation threshold for a stationary point in the configuration space. It is worth noticing that while this organization is at the heart of the mechanism of dynamical transition, there is no sign in the Gibbs measure that reveals this structure.

One might wonder if such an organization of stationary points is also found in the KA model. In order to investigate this point we have studied the number of blocked states at fixed overlap with a generic blocked state introducing in the auxiliary model a term $N(\epsilon/\beta_{aux})[q(\{n_i\},\{n_i^0\})-q]^2$, which for large ϵ constrains the configurations to have the desired overlap with the reference configuration. In the simulations the value $\epsilon=50$ proved to be effective to get the desired values of the overlap for all densities. We performed a simulated annealing of the model and we extracted the zero temperature entropy from thermodynamic integration of Eq. (1).

In Fig. 3 we show the entropy as a function of the overlap for different values of the density. It is apparent from the figure that both above and below the transition the curves behave qualitatively in the same way, with an entropy as a function of q which departs from zero regularly at $q=1$. This indicates that the structure of the blocked states does not change as we cross the transition. In particular, this shows that differently from the mean field spin glass case, the apparent dynamic transition in this model is not linked to a change of geometrical organization of the blocked states.

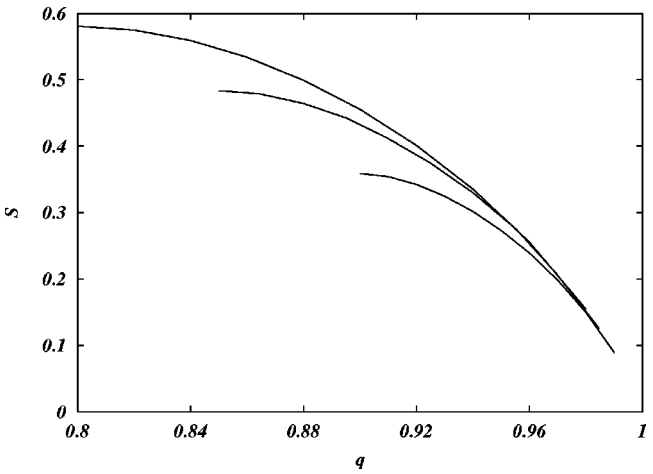

FIG. 3. The entropy of the blocked states as a function of q for densities (from top to bottom) $\rho=0.8,0.85,0.9$.

IV. CONCLUSIONS

In this paper we have investigated the mechanism which leads to vitrification in kinetic lattice gases, in comparison with the one responsible for glassy phenomena in mean field models with random Hamiltonian.

We have found that in the low density phase, despite the trivial character of density correlation implied by the equilibrium distribution, as it happens in supercooled liquids the dynamics has a heterogeneous character. The four-point correlation function displays a maximum as a function of time that grows as a power of $\rho-\rho_c$, and the dynamics remain correlated for times which also grow as a power of the same quantity.

We have shown that the blocked states are unstable and play no role in the low density phase, while they are stable and act as attractor in the high density phase. Furthermore, we have investigated if this stability property corresponds to a different organization of the blocked states in phase space, with negative result. In both dynamical phases (low and high density), one finds blocked states at all distances from any blocked state.

Then, we can conclude that despite the similarities in the dynamics, the glassy phenomena in kinetic models, at least at the level of the phase space organization, are very different from the ones found in systems with a complex energy landscape.

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