Defect diffusion and cooperative dynamics in models of glasses

Biroli G.[a] and Toninelli C.[c]

[a]SPhT, CEA/Saclay-Orme des Merisiers, F-91191 Gif-sur-Yvette Cedex, FRANCE;

[c]Laboratoire de Physique Théorique de l'ENS, 24 rue Lhomond 75231 Paris Cedex, FRANCE

ABSTRACT

We present some of our work (done in collaboration with D.S. Fisher) on Kinetically Constrained Lattice Gases focusing on the Kob and Andersen's simple lattice models (KA) for the dynamics of structural glasses. In these systems, although the particles have only hard core interactions, the imposed constraint that they cannot move if surrounded by too many others causes slow dynamics. A very rich dynamical behavior emerges from the simple kinetic rules introduced by KA. Finite dimensional KA models "almost" have a dynamical phase transition: such a transition exists on Bethe lattices and it is replaced by a crossover in finite dimensions. The dominant processes that destroy this putative "mean-field" transition involve cooperative rearrangements of regions, called defects, whose size diverges in the high density limit leading to a physical behavior reminiscent of fragile glass-forming liquids.

Keywords: Glass Transition, Jamming Transition, Kinetically Constrained Lattice Gases.

1. INTRODUCTION

The glass transition, whether a true transition or a sharp crossover in the dynamics, is one of the longest standing unsolved puzzles in condensed matter physics. Many liquids, when cooled fast enough in order to avoid crystallization, appear to freeze into an amorphous solid-like structure. In this metastable regime the time scale for structural relaxation increases dramatically as the temperature is lowered; materials are conventionally called glasses when this time becomes larger than experimentally accessible time scales. In *fragile liquids* the relaxation time increases much more rapidly than Arrhenius.[1] Near the glass "transition", the relaxation processes become complicated, often characterized by stretched exponential decay of temporal response functions,[1] and spatial heterogeneities appear in the dynamics in both experiments[2] and numerical simulations.[4–8]

In spite of a great deal of theoretical effort, a real understanding of these and related phenomena is still lacking: indeed, the most basic issues are still unresolved: Is the rapid slowing down due to proximity to an equilibrium phase transition of some kind (albeit perhaps in a restricted part of phase space)? Or is the underlying cause entirely dynamical? What is the physical mechanism behind the super-Arrhenius behavior? What is the origin of the spatial heterogeneity observed in the dynamics?

Theoretical developments in this field have been hampered by a shortage of models that capture at least some of the features believed to be essential, yet are simple enough to analyze. In other fields of statistical physics, such models have played vital roles, leading to understanding, to sharpening of questions, and to development and analysis of improved models. One of the few classes of such models for glasses are the *kinetically constrained* lattice models; a subset of these is the focus of this paper. The basic Ansatz of kinetically constrained lattice models is that the key to the glass transition lies in the geometrical constraints on the rearrangements of the atoms or molecules and the effects of these on the dynamics; static correlations, beyond those present in dense liquids, are assumed to play no role. The simplest such systems are ones in which the energetics plays no role beyond hard core repulsion but there are kinetic constraints on the motion. For reviews see.[10,11]

In addition to their potential as models of glass transitions, kinetically-constrained lattice models are natural for granular media — another class of systems in which extremely slow dynamics has a rather sudden onset at densities well below close-packing.[12]

A particularly interesting class of models was introduced by Kob and Andersen (KA)[13]: in these lattice gases,

Send correspondence to G. Biroli. E-mail: biroli@spht.saclay.cea.fr

which have detailed balance, particles can move only if their local environment is not too constrained — the specific rules are given below. These models have very sluggish dynamics at high density and a phenomenology very similar to glass-forming liquids.
In[14,15] we have unveiled the physical origins of the glassy behavior of KA and generalized the results to other kinetically constrained lattice models. In the following we shall present some of these results showing that indeed these simple kinetically constrained models exhibit concretely some of the qualitative features conjectured by many to be the cause of the dramatic slowing down in structural glasses.

2. KINETICALLY CONSTRAINED LATTICE GASES

In the last twenty years there has been a growing interest in kinetically constrained lattice models. These were introduced as models for supercooled liquids close to the glass transition[9] and nowadays they are also studied as paradigm for general glassy systems (see[10] for recent reviews). Kinetically constrained models can be divided in two large classes: spin and particle models. In the following we shall focus mainly on particle systems, also called Kinetically Constrained Lattice Gases (KCLG) and we shall only briefly discuss the spin models (since they are in general quite similar to their lattice counterparts).
KCLG can be viewed as a generalization of the standard non interacting lattice gas, also called simple symmetric exclusion process in which only nearest neighbor jumps are allowed provided the constraint of having maximum one particle per site is verified. The important new ingredient of KCLG is encoded in the choice of the jump rates of particles that are different from zero not only if the constraint of having maximum one particle per site is verified but *also* if some additional constraint is verified, hence the name kinetically constrained. The choice of this constraint, i.e. of the jump rates, was originally devised in order to mimic the cage effect, that might be at the heart of the glassy behavior and the slow dynamics of glass forming liquids. Indeed a molecule in a dense liquid is typically trapped in a cage created by surrounding particles (see[3] for a visual experimental example) and this takes place in the regime of temperature and density at which the dynamics slows down dramatically.
Another important feature of KCLG (at least of the simplest ones) is that the rates are chosen in order to satisfy detailed balance with respect to the uniform measure on all the configurations with the same particle density. Note that this means that the stationary equilibrium measure corresponds to a zero Hamiltonian. Thus there are no static interactions beyond hard core and an equilibrium transition cannot occur. Despite this trivial thermodynamics, the dynamics is very sluggish at high density and phenomenologically similar to the one of glassy systems. For example, as discussed in,[10] numerical simulations have shown that some KCLG display super-Arrhenius behavior, non-exponential equilibrium relaxation, aging phenomena in the off-equilibrium dynamics and dynamical heterogeneity.

2.1. The Kob-Andersen model

One of the most studied kinetically constrained models, displaying a whole phenomenology similar to glass forming liquids,[10] is the Kob-Andersen model.[13] This is a single component lattice gas with no static interactions other than hard core exclusion and dynamics given by a continuous time stochastic process. Each particle attempts, at a fixed rate, to move to a randomly chosen empty neighboring site; *but* the jump is allowed only if both before and after the move the particle has no more than some number, m, neighboring particles. This corresponds to *vacancies* moving only if the initial and final sites have at least $s = z - m - 1$ neighboring vacancies, with z the coordination number of the lattice. Since this dynamics satisfies detailed balance, the trivial distribution that is uniform over all configurations with a fixed number of particles is stationary: thus there can be no equilibrium transition. Nevertheless, the dynamics at high density displays all the glassy properties mentioned above.[13,16,17] Indeed, for a three dimensional cubic-lattice with $s = 2$, fits of the self diffusion coefficient of a tagged-particle, D_S, and of the relaxation timescale strongly suggest a dynamical glass transition at $\rho_c \simeq 0.881$, above which D_S appears to vanish and the structural relaxation time to diverge.[13] We have shown by rigorous and physical arguments that, instead, this model remains ergodic with a strictly non zero diffusion coefficient at any density less than one.[14,21] However, as shown in[14] and discussed below, at high density the dynamics becomes intrinsically collective and extremely slow.

2.2. Independent defect diffusion

As explained in[10] and discussed in the next section, the majority of KCLG are characterized at high density by the existence of "defects" that are the analog of vacancies for the simple non interacting lattice gas. Note that the word "defect" is not related to the existence of structural or topological defects and probably a better word, used in our paper,[14] would be mobile region. However, since this terminology is used in the recent review,[10] we are also going to use to it in the following.
The slow dynamics can be explained simply in terms of defect motion: the defects perform independent random walks and substantial structural relaxation or movement of a tagged particle takes place only when a defect passes by. So the high density dynamical behavior is encoded in the properties (size, timescale for motion, density, ...) of the defects. As an example, we show below a simple argument that allows one to obtain the correct density dependence of the self-diffusion coefficient D_S in the approximation of independent defects. Note that D_S is one of the main quantities studied numerically and experimentally for glassy systems.
Call ρ_d the density of defects and τ_d the timescale on which defects move of one step. The self-diffusion coefficient D_S of a tagged particle is expected to be proportional to the inverse of the time τ_p on which each particle moves of one step. On the timescale τ_d the number of particles that have jumped is of the order $V\rho_d$ where V is the total number of sites. Thus we find, in dimension larger than one:

$$\frac{\tau_p}{\tau_d} V\rho_d \propto V\rho. \tag{1}$$

As a consequence, at density close to one, we get $D_S \propto \rho_d/\tau_d$. Note that this results can indeed be rigorously proven in many cases,[21] called non cooperative in the following.
Remark also that for simplicity we didn't discuss how the size of the defects changes with density because in the model we are going to discuss either this doesn't change with density or it gives a subleading contribution to D_S.
As a simple example, one can consider the non-interacting lattice gas. In this case the vacancies are the defects. Thus, in the limit $\rho \to 1$, $\rho_d \propto (1-\rho)$ and $\tau_d \propto O(1)$, hence, $D_S \propto (1-\rho)$, a well known result. In next section we shall go through more interesting examples that will allow us to show how non trivial defect properties, and hence dynamic properties, can emerge in KCLG.
We conclude this section with two important remarks. First, kinetically constrained *spin* models also can be described in terms of defect motion.[10] However, in this case, defects interact much more because the dynamics does not conserve particle density and it has been shown, at least for the one spin facilitated Fredrickson-Andersen model, that the defects cannot be considered non-interacting in less than four dimensions[18] (see below for a more detailed discussion).
Finally, we want to stress that the explanation of the slow dynamics of glass forming liquids in terms of defects motion is a long story that, to our knowledge, goes back to Glarum[19] in the '60, i.e. well before the first kinetically constrained models were introduced, and that it have been pursued until now[20] with different assumptions on the dynamic properties of these defects. However, an important outcome of the analysis of KCLG, that would have been impossible to guess a priori, has been to show how highly non trivial defect properties leading to a cooperative slow glassy dynamics can emerge from very simple dynamical rules.[10,14]

3. WHAT IS A DEFECT?

In this section we shall discuss, going through different examples, the properties of defects and how they arise from the kinetic constraints.
A first classification differentiate simple non cooperative cases in which a finite cluster of vacancies can move in an otherwise completely filled lattice from cooperative ones where the number of vacancies involved in a defect increases and diverges approaching the zero density vacancy limit.

3.1. Simple non cooperative cases

The first and simplest example of non cooperative case is the simple non interacting lattice gas discussed previously in which the defects are simply the vacancies.
A more instructive case is the KA model with $s = 1$ on the triangular lattice represented in figure 1. Note that for this choice of the lattice two neighboring sites share a common third neighbor. Furthermore, as already

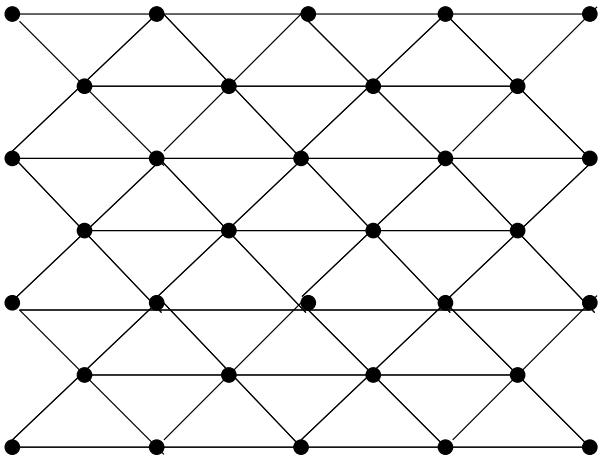

Figure 1. The triangular lattice

noticed, the KA rates reformulated in terms of vacancies correspond to the rule that a vacancy can move only if the initial and final sites have at least s neighboring vacancies, where $s = 1$ in the case we are considering. Therefore any of the two vacancies of a neighboring couple can move to the common third neighbor. In other words a couple of neighboring vacancies is a finite size freely mobile cluster, which we call "defect". See figure 2 for a visual explanation of how a defect move. The density of such defects is of the order $(1-\rho)^2$ when $\rho \to 1$ and they move on a timescale which is of order one. Applying the simple formula obtained in the previous section this implies a self-diffusion coefficient for a tagged particle that scale as $(1-\rho)^2$ when $\rho \to 1$.
Other examples are: a KA $s = 1$ model on a face centered cubic lattice with links between nearest and next nearest neighbor sites. This is a sort of a 3D generalization of the triangular lattice case considered above in which, again, any of the two vacancies of a neighboring couple can move to the common third neighbor. Thus a couple of neighboring vacancies is a "defect". Another example is a KA $s = 2$ model on a body centered cubic lattice with links between nearest, next nearest and next next nearest neighbor sites. In this case a defect consists in three vacancies belonging to the same tetrahedron. Thus the defect density and the self diffusion coefficient of a tagged particle scales as $(1-\rho)^3$ when $\rho \to 1$.
More generally, in non-cooperative cases, one can identify a defect with a finite cluster of vacancies that can move in an otherwise completely filled lattice. If the defect is formed by q vacancies, the self-diffusion coefficient as well as the inverse relaxation timescale are expected to scale as $(1-\rho)^q$ when $\rho \to 1$. A resulted that we have rigorously proved in.[21]
We conclude this section with a remark about the hypothesis that defects do not interact. Although this is certainly true in the simple non interacting lattice gas, already for the simple case of a KA $s = 1$ on a triangular lattice one may have doubts since when two defects, i.e. two couple of nearest neighbor vacancies, meet they certainly interact with a possible annihilation of one of the two defects. More specifically, when defects A and B meet, one of the two vacancies of, say, defect A can move, thanks to the neighboring vacancies of defect B to a next nearest position with respect to the other vacancy in defect A. As a consequence, when defect B diffuses away, the two vacancies that formed defect A are now no more nearest neighbors, i.e. defect A has been annihilated. A similar process can create one defect starting from two next nearest neighbor vacancies when a defect passes by. Once defects start to interact with annihilation and creation mechanisms one can wonder if physical results obtained with the *independent* defect hypothesis hold. The answer is that, from the properties of random walks, one expects that at least for dimension larger than four these results should hold. As already pointed out, we have proven[21] that the heuristic result (1) on the self-diffusion coefficient based on the *independent* defect hypothesis is correct[21] in dimensions larger than one. So that is likely that this hypothesis is indeed correct for KCLG in dimension larger than one.
However, in the case of the Fredrickson-Andersen one spin facilitated model, a kinetically constrained *spin* model, renormalization group analysis as well as numerical simulations show that indeed this hypothesis breaks down.[18]

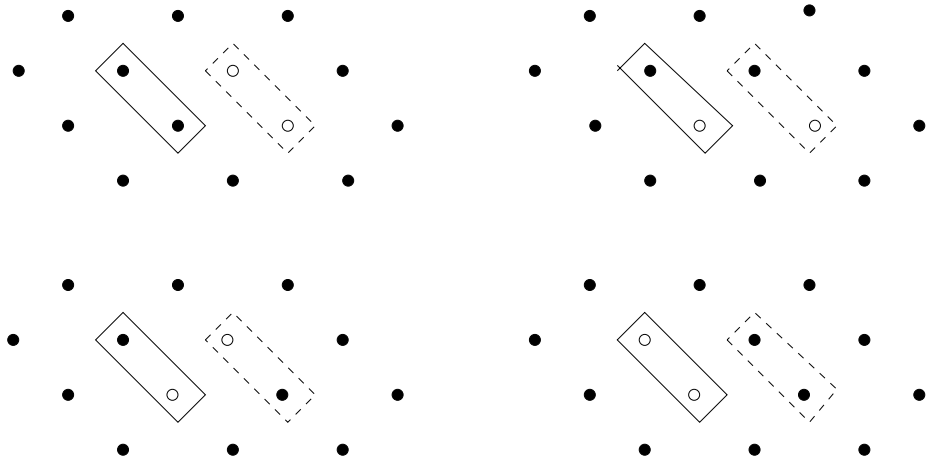

Figure 2. Sequence of moves which allow the displacement of a couple of neighboring vacancies. Circles denotes empty sites, filled dots stand for occupied sites

A way to reconcile these two apparently contrasting results is noticing that in the case of particle models, because the density of particles is conserved, even if a defect is destroyed, two vacancies remain in the annihilation region so that the annihilation (as well as the creation process) is strongly inhibited because one cannot have too many annihilations (or creations) in the same region. Instead, in the case of spin models, since the dynamics does not conserve the density (the magnetization in spin language), annihilation (or creation) is not inhibited at all in a region in which annihilation (or creation) has taken place previously.

3.2. Cooperative cases

For simplicity we focus on the simple KA $s = 1$ on a square lattice case. This is the simplest case of cooperative KCLG.[14] In this case one cannot construct defects formed by vacancies that can freely move in an otherwise completely filled lattice.[14] This can be proved simply by noticing that any finite cluster of vacancies can never overcome a completely filled double row *. Thus, to understand what a defect is one has to find minimal configurations of vacancies that can move inside the lattice using the other vacancies. For example, consider a l by l square filled by particles but with all the boundary sites empty (right part of fig. 4). It's easy to check that if this configuration, that we call *framed* in the following, has at least two vacancies on the line just above the top edge then this framed configuration can move up of one lattice spacing. If l is large enough the probability to have these two vacancies on each of the l lines above is of the order one. A simple calculation gives $l = \xi \sim \ln(1/(1-\rho))/(1-\rho)$. Thus, framed configurations can move and diffuse (in a random evolving media formed by the other vacancies) when $l > \xi$. The probability to have a framed configuration is however extremely small for large l, of the order $(1-\rho)^{4l}\rho^{l}$. Indeed one shouldn't focus on just framed configurations but on all the configurations of the l by l square, called *frameable* in,[14] that through a sequence of allowed moves can reach the framed configuration. A defect can be in any of the frameable configurations and the framed configuration is just the gate or the bottleneck in configuration space that has to be reached dynamically in order to move of one step. See fig. 3 for an example of defect.

Now that the defects has been defined let us discuss their two fundamental properties: their density and their typical timescale for movement.

To obtain the defect density one has to know what is the probability that an l by l configuration is frameable. In order to get this quantity[14] we focus on a way to construct frameable configurations based on the following iterative procedure: an l by l frameable configuration that has at least two vacancies externally adjacent to each of its sides is also an $l+2$ by $l+2$ frameable configuration, because it can be first transformed in a framed configuration and then expanded, see fig. 4. Thus, starting from a two by two frameable "nucleus" of vacancies,

*We take periodic boundary conditions.

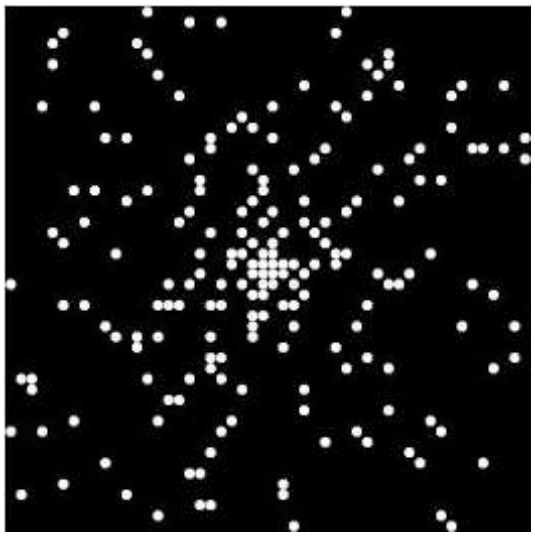

Figure 3. A defect of linear size 50 lattice spacing in the two dimensional KA $s = 1$ model.

one can thus grow an l by l frameable configuration if the requisite vacancies are present in each concentric shell. The probability that this occurs is $P_l(\rho) = (1-\rho)^4 \prod_{m=2}^{l/2}[1-\rho^{2m}-2m\rho^{2m-1}(1-\rho)]^4$ which converges to a non-zero probability, $P_\infty(\rho)$ in the infinite l limit. For small vacancy densities, $P_\infty(\rho) \simeq e^{-2\hat{K}_F/(1-\rho)}$ with $\hat{K}_F \simeq 4.48$. Moreover, $P_l(\rho)$ depends weakly on l for $l > \xi \sim \ln(1/(1-\rho))/(1-\rho)$; ξ is thus the *core* size of frameable regions. Note that P_l is the probability that a frameable square can be constructed around a nucleus at a *fixed* position. To get the defect density inside a system of size L one has to consider all the $O([L/\xi]^2)$ possible positions of a nucleus. As it can be proven,[14] defects with nuclei separated by more than a core diameter are roughly independent events, thus the number of defects in the system is simply $(L/\xi)^2 P_l(\rho)$, i.e. the defect density is $(1/\xi)^2 P_l(\rho)$[†].

We now turn to the typical timescale on which defects move. Since all frameable configurations are equiprobable this is proportional to $\exp(\Delta S)$, the ratio of the number of accessible (frameable) configurations of the core to the number in the most severe bottleneck in configuration space.[15] The worst case scenario in which the bottleneck corresponds to a *single* configuration, the framed one, leads to $\Delta S = S_{\rm total} \simeq \ln(l!)^4$ since the total number of frameable configuration is roughly $l!^4$. However, as explained in[14] the bottleneck is not so tight, i.e. defects do not have necessary to go trough the framed configurations in order to move. Analytically and numerically we have found $\log \tau_d \propto \sqrt{l}$.[14]

Another important defect property that we need to know is the typical size of the defects responsible for structural relaxation and diffusion. Since increasing l the defect density decreases and the timescale for defect motion increases one has just to focus on the smallest value of l which guarantees defect diffusion, i.e. $l = \xi \propto \log(1-\rho)/(1-\rho)$ as we have explained previously.

Finally, let us remark that one can object to the content of previous paragraphs that all that has been obtained is just one possible way for the system to relax, one would like to know the fastest one. Indeed changing slightly the definitions of defects[14] we identified the fastest way for the systems to relax and we checked our results against numerical simulations, see below. Briefly, all qualitative results explained above remains the same but they change quantitatively. Indeed the value of $\hat{K}_F$ entering in the defect density is changed to $K_F \propto 0.55$.

So, at the end, we have obtain a picture of the KA model in which, at high densities, vacancies will typically be far apart or in small clusters that cannot move. However vacancies and particles can move within the defects. And these defects are themselves mobile because they are likely to find vacancies on *all* the ξ successive line segments needed for them to move in a given direction. A generic particle cannot move substantial distances

[†] Note that in principle this argument leads just to an upper bound. However in[14] we have also obtained a lower bound which matches with this upper bound for optimal defect (see below in the text).

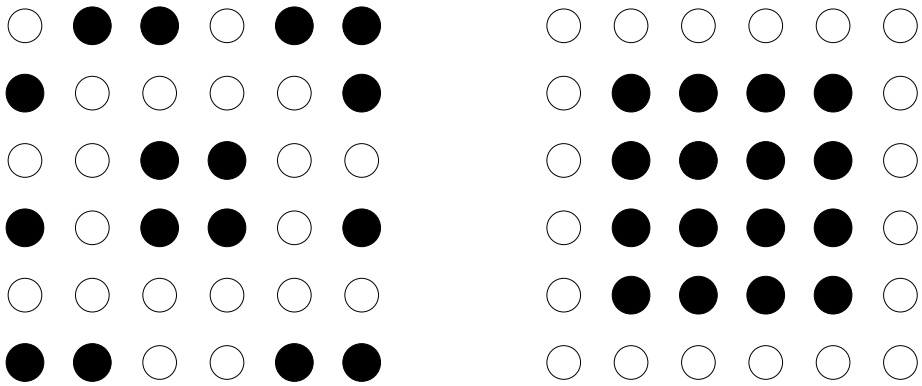

Figure 4. On the left there is a 4 by 4 framed configuration with two vacancies (white circles) adjacent to each side. After moving the external vacancies at the corners the framed square can be expanded to the 6 by 6 framed configuration on the right.

except when a mobile core passes by; assuming independent core motion a tagged particle will thus diffuse with $D_S \sim \rho_d/\tau_d$. Since $\rho_d << 1/\tau_d$ the leading contribution to D_S arises from the low density of mobile regions rather than the long time needed for motion within them. Thus, to leading order in $(1-\rho)^{-1}$, $\ln D_S \approx 2K_F/(1-\rho)$ for the square lattice model with $s=1$. Numerical simulations at high densities fit this form well, see fig. 5: in particular $\lim_{v\to 0} v \ln D = 2K_F \cong 0.9 - 0.95$ *cf* the predicted $2K_F \cong 1.1$.
Analogous results can be obtained for KA model on hypercubic lattices in any finite dimension d and for different choices of $s > 0$.[14] Again, one can identify cooperative defects which guarantee a finite self diffusion coefficient at any density $\rho < 1$ which vanishes for $\rho \to 1$ faster than any power law. The dependence on ρ is again related to the density ρ_d of such defects, which in the general case decreases for $\rho \to 1$ as $\rho_d \propto 1/\exp^{\circ s} \frac{C(d,s)}{(1-\rho)^{d-s}}$ with $\exp^{\circ s}$ the exponential iterated s times.[14] In particular, for the three dimensional case with $s=2$ originally considered by Kob and Andersen, we find $\rho_d \propto 1/\exp\exp K/(1-\rho)$ with K a positive constant yielding $\ln\ln D_S^{-1} \propto 1/(1-\rho)$, a result consistent with a finite size scaling analysis.[8]

4. AVOIDED TRANSITION AND DYNAMICAL CROSS-OVER

As discussed in the previous section, for KA model on hypercubic lattices we have identified cooperative defects which are the physical mechanism for the very sluggish dynamics at high density. Their size, as well as their typical timescale, increases with density and diverges at $\rho = 1$. Having understood the high density regime it's natural to investigate what happens in an intermediate regime, i.e. when the characteristic size of the defects becomes of the order one. In order to do that it's useful to think how defects of size of the order one can move and why they have to grow at high density. Let us focus for simplicity on the square lattice case with $s=1$. In this case one can directly check that a cluster of three vacancies can move along a network of empty sites that are linked no more weakly than via second neighbors along axes or diagonals, so they are a moving defect of size of order one. Let p_{3P} be the critical density for third neighbor percolation, (namely two particles are connected if they are first, second or third neighbors one to the other). If the density of vacancies is above such threshold, i.e. $1-\rho > p_{3P}$, there exists with unit probability an infinite percolating cluster of vacancies on which a cluster of three vacancies can move in a non-cooperative way. However such defects, at variance with single vacancies in the normal lattice gas or the couples of vacancies on the triangular KA model with $s=1$, cannot move freely into an otherwise totally filled lattice. They need a particular underlying structure of vacancies: the percolating cluster discussed above. The motion of these non cooperative defects gives a power law contribution to the diffusion coefficient because it is roughly proportional to their density, the probability of being on the infinite cluster and the self diffusion coefficient on a percolating cluster. These last two quantities vanish as a power law at the percolation transition that, running simulations using the algorithm of Hoshen and Kopelman,[22] we have found equal to $p_{3P} \simeq 0.29$.
Therefore, coming from low density, we expect a first regime in which the diffusion slows down because the

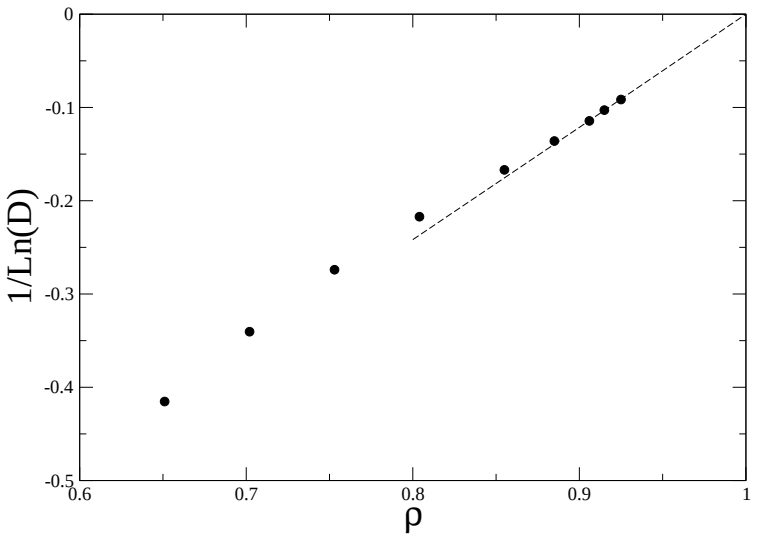

Figure 5. $(\ln D)^{-1}$ as a function of ρ for a KA on 400 by 400 square lattice with $s = 1$. Straight line shows $\ln D_S \propto 1/v$ behavior.

second–neighbor vacancy percolation giant cluster, on which the three–vacancy elements (the defects) can move, shrinks. Afterwards, for $\rho > 1 - p_{3P}$ (or slightly higher due to small scale processes), the mobile elements have to grow in order to remain mobile and they become continuously the cooperative defects discussed in the previous section. In two dimensions such crossover between non-cooperative to cooperative dynamics is not sharp enough in order to determine an unambiguous power law of $\rho - \rho_{3P}$ in the vicinity of ρ_{3P}.
The above arguments can be generalized to other cases of KA, with the crossover density determined by more complicated types of percolation. If the crossover is sufficiently sharp–which we expect to be true at sufficiently high spatial dimensions–one should observe a substantial range of critical dependence of D_S near an apparent transition. This is a possible explanation of the numerical results for the original cubic case with $s = 2$, where for more than three decades D_S is well fitted by a power law vanishing at $\rho \sim 0.881$.[13]
We will come back in the end of next section on the meaning of such crossover and on its relation with the study of *activated processes* for supercooled liquids.

5. THE BETHE LATTICE GLASS-JAMMING TRANSITION

In this section we consider the KA model on Bethe lattices. In this case we show that an ergodic/non–ergodic transition occurs at a finite density ρ_c. At low enough density relaxation is due to the motion of finite size defects (as on hypercubic lattices), but at high density on such graphs it is not possible to construct large density dependent defects that cooperatively move. In other words the dynamical crossover which occurs on hypercubic lattices is replaced by a true dynamical transition on these graphs.
Let us first recall the definition of a Bethe lattice. Bethe lattices are random simple graphs with N sites and fixed connectivity $z = k + 1$, which crudely approximate high–dimensional or high–coordination–number lattices. The tree–like local structure of such graphs allows analytic calculation trough the solution of recursive equations. Consider a Bethe lattice with connectivity $k + 1$. KA model is defined as previously and now we focus on $0 < m < k$ and $s = k - m$. As usual, one arranges the lattice as a tree with k branches going up and one going down. Consider one node, and define following events:

1. the node is occupied by a particle which cannot move up even if the site below it is empty.
2. the node is empty but a particle can never move onto it from below.
3. the node is occupied by a particle which can only move up if the node below it is empty.

4. none of the above.

By using the tree–like structure, we have written iterative equations for the probabilities P_1, P_2, P_3, P_4 and, analyzing them, we have shown (see[14,15]) that a dynamical transition takes place for all the choices of k and s with $s > 0$ ($s = 0$ corresponds to the trivial lattice gas case, for which no transition takes place). Indeed, there exists a critical density $\rho_c < 1$ such that for $\rho < \rho_c$ the probability P_1 is zero and for $\rho > \rho_c$ it is positive. Such dynamical transition is associated with the emergence of an infinite cluster of permanently blocked particles, as can be proved by identifying the transition with the percolation transition for a suitably defined *bootstrap procedure* (see[14,15]) ‡. Furthermore, for $k = s$ such transition is continuous, while for $k < s$ $P_1(\rho_c) > 0$, i.e. the transition has a first order character. In this case, above ρ_c, $P_1(\rho) - P_1(\rho_c) \sim \sqrt{\rho - \rho_c}$, with a singularity indicative of diverging length and time scales. The KA dynamical transition on this Bethe lattice has therefore both critical and "first order" characteristics. Interestingly, such features are analogous to those for the dynamical transition in infinite-range *quenched random* p-spin models, conjectured to be related to the glass transition.[24,25] An interesting hypothesis is that such mean field transition, which is due to the existence of infinite barriers, should be substituted in real systems by a crossover between a power law to an *activated regime* related to the super-Arrhenius behavior of fragile liquids.[24] However, no systematic derivation has been presented in the literature neither in the finite dimensional case or for the finite-size completely connected systems. If one takes seriously the analogy between the dynamical transition of infinite-range *quenched random* p-spin models and the Bethe lattice KA transition then our results for the KA show, in a specific example, both the mechanism which induces the mean field dynamical transition (the emergence of infinite clusters of forever blocked particles) and the cooperative processes (the motion of large density dependent cores) which allow diffusion and structural relaxation for finite dimensional systems even in the high density regime, i.e. after the mean-field transition. The behavior of the relaxation timescale, which increases extremely faster as a function of $1 - \rho$ in this regime, is indeed reminiscent of the super-Arrhenius scaling of the structural relaxation timescale of fragile liquids close to the glass transition.

6. CONCLUSION

We have shown that the simple kinetically constrained models introduced by Kob and Andersen exhibit, in a concrete manner, some of the qualitative features that many have conjectured to be the underlying cause of the dramatic slowing down in structural glasses. In particular, the finite-dimensional models "almost" have a dynamical phase transition: such a transition exists on Bethe lattices and simple percolation arguments suggest that it is replaced by a crossover — which could be very sharp — in finite dimensions. The dominant processes that destroy this putative "mean-field" transition involve cooperative rearrangements of regions, called defects, whose size diverges in the high density limit; these yield a non-vanishing self-diffusion coefficient at all densities. Nevertheless, the length and time scales of these processes grow extremely rapidly at high densities.
One of the most interesting outcome of our study is to show how very interesting and unexpected defect properties, leading to a dynamics reminiscent of the one of glass-forming fragile liquids, can emerge from very simple dynamical rules.

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‡These results hold also for Bethe lattices with *finite size loops*,[15] i.e. for the so called pure Husimi trees[23] and for Bethe lattices where single sites are replaced by $L \times L$ squares (these interpolate among the Bethe lattice ($L = 1$) and the square lattice ($L = \infty$) case).

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