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Universal and nonuniversal properties of a lattice gas model with kinetic constraints

A. Imparato *, L. Peliti [1]

Dipartimento di Scienze Fisiche and Unità INFM, Università di Napoli ''Federico II'', Mostra d'Oltremare, Pad. 19, I–80125 Naples, Italy

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Abstract

We study by numerical simulation the Kob–Andersen (KA) model of a lattice gas with kinetic constraints on a face-centered cubic (FCC) lattice, both in its canonical and in its grand-canonical version, and for different dynamical rules. The model exhibits a dynamical transition at a threshold value of the density, where the diffusion constant vanishes as a power law. We confirm that the corresponding exponent is independent of the details of the dynamics, while the threshold density is nonuniversal. On the other hand, the fluctuation–dissipation ratio X appears to be nonuniversal. © 2000 Elsevier Science B.V. All rights reserved.

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The Kob–Andersen (KA) model is a very simple model of a structural glass which, in spite of its simplicity, exhibits a remarkably wide range of genuinely glassy properties [1]. Its equilibrium properties are trivial (being those of an interaction-free lattice gas), but it exhibits a purely dynamical transition as a function of density. As the density ρ approaches a threshold value ρ_c from below, the diffusion constant D of the particles forming the gas vanishes as

$$D \sim |\rho - \rho_c|^{\beta}. \quad (1)$$

On a simple cubic (SC) lattice of size 20^3, the simulations performed by Kob and Andersen yield $\rho_c = 0.88$ and $\beta = 3.1$. The arguments reported by [1] suggest that the threshold density reaches $\rho_{max} = 1$ in the thermodynamic limit. The approach is however so slow (like $\ln\ln L$, where L is the size of the system) that it is warranted to take the transition as a bona fide one for finite systems.

It is tempting to assimilate the vanishing of the diffusion constant to a (purely dynamical) glassy transition. In fact, Kurchan et al. [2] have slightly generalized the model, allowing the system to ex-

* Corresponding author. Present address: Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Abteilung Theorie, D-14424 Potsdam (Germany).

E-mail addresses: imparato@mpikg-golm.mpg.de (A. Imparato), peliti@na.infn.it (L. Peliti).

[1] Associato INFN, Sezione di Napoli.

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change particles with a reservoir via an open boundary. They were able therefore to perform numerically the analogs of cooling and quenching experiments, obtaining distinctly glassy behavior. In particular, the outcome of the quenching experiment was an aging behavior, exhibited, e.g., by the two-time correlation functions, which could be analyzed via a simple mean-field theory [3]. In this case, it appears that the aging behavior is a consequence of the fact that the density approaches its critical value as a power law in time. Other nontrivial aspects of aging behavior, like the presence of a Fluctuation–Dissipation Ratio (FDR) smaller than one, have also been numerically exhibited [4].

The power-law dependence of the diffusion constant as a function of the density is reminiscent of a critical point. If the analogy holds water, we would expect the exponent β to be independent of the details of the dynamics, while the threshold density ρ_c depends on them. This conjecture is hard to check in the original model, which does not allow enough parameter freedom. By putting the model on a face-centered cubic (FCC) lattice, we provide us with an extra parameter which allows for a limited test of universality. We are thus able to confirm the universality of the exponent β, while the threshold density ρ_c and the FDR turn out to be nonuniversal.

The KA model is defined as a lattice gas model of N sites, in which particles can evolve according to the following dynamical rules. At each step, a particle and one of its neighboring sites are chosen at random. The particle moves to the site if the following conditions are all satisfied:

1. The site is empty;
2. The particle has m or fewer occupied nearest neighbor sites;
3. In its new position, the particle would have m or fewer occupied nearest neighbor sites.

With these rules, detailed balance is satisfied and all possible configurations have the same weight.

In the original version, the lattice is isolated from the environment and the number M (and thus the density $\rho = M/N$) of particles is conserved. This is the 'canonical' version of the model. Kurchan et al. [2] introduced a 'grand canonical' version by allowing particle exchange with a reservoir (at chemical potential μ) on a single two-dimensional surface. In this version, the above rules are supplemented by the following rule:

1. A site on the surface is chosen at random;
2. If the site is empty, a new particle is added;
3. If the site is occupied, the particle is removed with probability $e^{-\mu}$, where $\mu > 0$ is the chemical potential.

The equation of state giving the equilibrium density ρ_{eq} as a function of the chemical potential μ is

$$\rho_{eq}(\mu) = \frac{1}{1+e^{-\mu}}. \tag{2}$$

We have mentioned above the results obtained by Kob and Andersen [1] on the SC lattice, with the threshold m set to 3: the diffusion coefficient D vanishes as ρ approaches ρ_c as shown in (1), with the critical density ρ_c equal to 0.88 and the exponent β equal to 3.1. It is not feasible to check the universality of these results on a SC lattice, since 3 is the only reasonable value of m.

We have therefore defined the KA model on a FCC lattice, which has coordination number equal to 12, and we have used different values of m to check for the universality of the parameters ρ_c and β appearing in (1). We have evaluated the diffusion constant as a function of the density in the canonical version of the model. We have also evaluated the fluctuation–dissipation ratio (FDR) in the aging state after a quench in the grand canonical version of the model.

A quench can be realized in this model by a sudden compression, i.e., by letting the chemical potential μ increase suddenly from below to above the critical value μ_c defined by

$$\rho_{eq}(\mu_c) = \rho_c. \tag{3}$$

Following a quench at $t=0$, two-time correlation and response functions start exhibiting aging properties. Consider, e.g., the displacement autocorrelation function $B(t+t_w, t_w)$ defined by

$$B(t+t_w, t_w) = \frac{1}{M}\sum_{i=1}^{M}\left\langle |\boldsymbol{r}_i(t+t_w) - \boldsymbol{r}_i(t_w)|^2 \right\rangle. \tag{4}$$

It turns out that, if t and t_w are large enough, this function depends on t/t_w rather than on $t-t_w$, as would be the case at equilibrium. In Ref. [3], this behavior is connected to the power-law decay of the average diffusion constant following a quench.

Following the method developed in Ref. [4], we consider the response of the system to a perturbation of the form

$$H_\epsilon = -\epsilon(t)\sum_{i=1}^{M} \boldsymbol{f}_i \cdot \boldsymbol{r}_i, \tag{5}$$

where $\boldsymbol{f}_i = (f_i^a)$ is a random vector associated with each particle in the system, and

$$\epsilon(t) = \begin{cases} 0, & \text{for } t \le t_w, \\ \epsilon_0, & \text{for } t > t_w. \end{cases} \tag{6}$$

We choose $f_i^a = \pm 1$ for $a = 1,2,3$ and $i = 1,\dots,M$. In the presence of the perturbation, a move which displaces particle i by the vector $\delta \boldsymbol{r}_i$, if it satisfies all other criteria, takes place with probability $\min(1, \exp(\epsilon_0 \boldsymbol{f} \cdot \delta \boldsymbol{r}_i / T))$. Since only the ratio ϵ_0/T has physical relevance, we set $T=1$ without loss of generality. The integrated response function to this perturbation is defined by

$$\chi(t+t_w, t_w) = \frac{1}{3M}\sum_{i=1}^{M} \langle \boldsymbol{f}_i \cdot \Delta \boldsymbol{r}_i(t+t_w) \rangle, \tag{7}$$

where $\Delta \boldsymbol{r}_i(t)$ is the difference between the position of particle i at time t in the presence of a perturbation (5) applied between time t_w and time $t+t_w$, and the position reached in the absence of the perturbation.

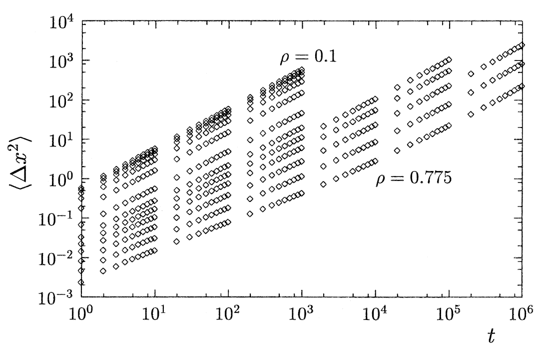

Fig. 1. Log-log plot of $\langle \Delta x^2 \rangle$ for different densities as function of the time, $m=6$. (From top left to bottom right: $\rho =$ 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.65, 0.675, 0.7, 0.725, 0.75, 0.775).

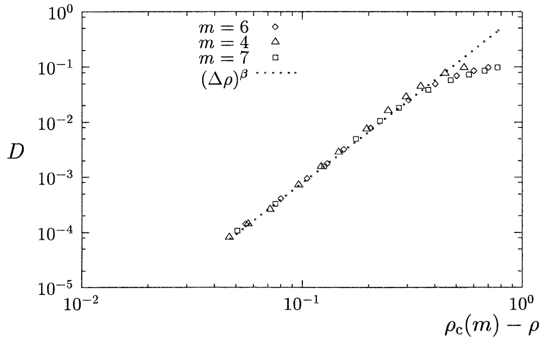

Fig. 2. Diffusion constant D versus $(\rho_c(m) - \rho)$ for $m = 4$, 6 and 7. The power law $D \propto |\rho_c - \rho|^\beta$, with $\beta = 3.1$, is represented by the dotted line.

The generalized Einstein–Stokes law [5,6] yields a relation between $\chi(t+t_w,t_w)$ and $B(t+t_w,t_w)$:

$$\chi(t+t_w,t_w) = \frac{\epsilon_0}{2}\int_0^{B(t+t_w,t_w)} \mathrm{d}B\, X(B). \tag{8}$$

If the FDT holds, $X(B)$ is equal to 1 and it follows that

$$\chi(t+t_w,t_w) = \frac{\epsilon_0}{2} B(t+t_w,t_w), \tag{9}$$

so that $\chi(t+t_w,t_w)$ is a linear function of $B(t+t_w,t_w)$ with slope $\epsilon_0/2$.

Sellitto [4] finds that, for the grand canonical KA model on a SC lattice, one has $X = 0.79$, so that the FDT is violated. He shows moreover that the FDR X does not depend on the supercritical value of μ_s used to perform the compression. This allows us to use a single value μ_s, for each value of m.

We use an FCC lattice with $20^3/2$ sites, with $m = 4$, 6, 7, and $\epsilon_0 = 0.05$. We have checked that with this value of ϵ_0 linear response theory holds.

Following the method used by KA, we determined the diffusion constant of our FCC model by measuring the mean square displacement $\langle \Delta x^2 \rangle$ of the particles as a function of the time. In Fig. 1, $\langle \Delta x^2 \rangle$ is plotted as function of the time, on a log-log scale, for $m = 6$ and for different values of the density. For low densities the curves have unit slope, which corresponds to normal diffusion, while

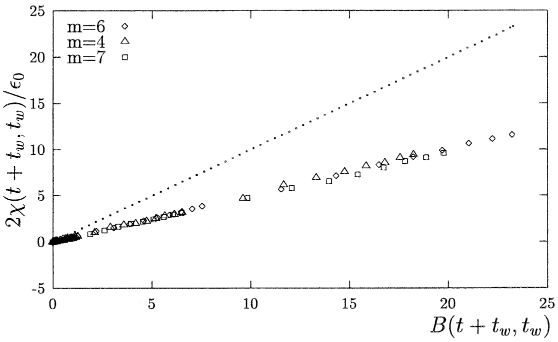

Fig. 3. Plot of $2\chi(t+t_\mathrm{w},t_\mathrm{w})/\epsilon_0$ versus $B(t+t_\mathrm{w},t_\mathrm{w})$ for $m=4$, 6 and 7, with $t_\mathrm{w}=10^4$. The dotted line has slope 1.

for higher densities the slopes become one only for long times.

Since

$$D=\frac{\langle \Delta x^2\rangle}{2nt}, \tag{10}$$

where n is a factor depending on the dimensionality, D can be obtained by fitting the long time behaviour of $\langle \Delta x^2\rangle$. Then, we fit the $D(\rho)$ data, for the different values of m, with a power law:

$$D=(\rho_c-\rho)^\beta, \tag{11}$$

finding the results reported in the following table:

m	ρ_c	β
4	0.647	3.10
6	0.806	3.10
7	0.876	3.09

In Fig. 2, we plot a data collapse of $D(\rho,m)$ versus $(\rho_c(m)-\rho)$ for the different values of m, and show that the laws we find well fit the data. While the values of β are in agreement with the one found by KA, the critical density ρ_c depends on m.

Our second aim is to test if the Fluctuation–Dissipation Ratio X is a universal quantity. We then reproduce the compression experiment of Ref. [4] in the FCC lattice. Namely, we prepare our system at the subcritical density $\rho_0<\rho_\mathrm{c}(m)$, then we compress it with a supercritical $\mu_\mathrm{s}>\mu_\mathrm{c}(m)$, measuring the response function (7), and the mean square displacement of the particles (4), after waiting $t_\mathrm{w}=10^4$ Monte/Carlo steps since the compression.

We plot $2\chi(t+t_\mathrm{w},t_\mathrm{w})/\epsilon_0$ versus $B(t+t_\mathrm{w},t_\mathrm{w})$ (Fig. 3) and fit the long-time data in order to obtain X, for the three values of m. The values of X are collected in the following table.

m	X
4	0.50 ± 0.01
6	0.507 ± 0.006
7	0.50 ± 0.01

These values are different from the one found by Sellitto in [4] $(X=0.79)$ for the SC lattice. However, they are equal to one another within the errors. One would thus obtain the strange result that X is a function just of the lattice, whereas it does not change with the critical density.

The behavior of the diffusion constant D as a function of ρ is reminiscent of critical phenomena: our results on the universality of β support this analogy and suggest that the singular behavior of D should be related to the existence of a diverging length, whose nature still has to be identified. On the other hand we do not expect to obtain the value of the fluctuation–dissipation ratio X via a simple approach, like the mean-field approach that has proved so successful in the derivation of the aging properties of $B(t+t_\mathrm{w},t_\mathrm{w})$ [3]. The KA model remains a surprisingly rich field for further investigations.

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