IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Granular compaction, random sequential adsorption and diffusional relaxation

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys. A: Math. Gen. 31 L425

(http://iopscience.iop.org/0305-4470/31/22/004)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.122
The article was downloaded on 02/06/2010 at 06:54

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. **31** (1998) L425–L433. Printed in the UK PII: S0305-4470(98)91522-0

**LETTER TO THE EDITOR**

# Granular compaction, random sequential adsorption and diffusional relaxation

Mário J de Oliveira†‖ and Alberto Petri‡§¶

† Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970 São Paulo, SP, Brazil

‡ Consiglio Nazionale delle Ricerche (CNR), Istituto di Acustica 'O M Corbino', Area di Ricerca di Roma—Tor Vergata, via del Fosso del Cavaliere, 00133 Roma, Italy

§ Istituto Nazionale di Fisica Nucleare (INFN), Sezione di Perugia, via A Pascoli, 06123 Perugia, Italy

Received 10 February 1998

**Abstract.** We introduce and perform numerical simulations of a lattice model for the compaction of a granular system based on the ideas of random sequential adsorption and diffusional relaxation. The lattice is composed by a given number of horizontal layers where nonoverlapping particles diffuse. Besides diffusion within its own layer a particle suffers a downfall to the layer below whenever there is enough space there. We restrict ourselves to the case of one-dimensional layers and particles that occupy $k$ consecutive sites. We observe time algebraic decay in the density of particles with exponents that are in several cases distinct from mean-field values.

A granular medium poured into a recipient and subject to mechanical perturbation displays a slow increase of density with time, the origin of this behaviour being the existence of space regions and local configurations that cannot be accessed unless to involve the motion of a large number of grains. A number of different approaches have been proposed in order to connect this observed slow compaction with effects of excluded volume and geometrical frustration [1] without reaching a unique conclusion concerning the temporal behaviour of the density change; experimental results obtained at the University of Chicago [2] are well described by logarithmic curves and the same behaviour is observed in some cellular automata, such as the tetris-like model of Caglioti *et al* [3], the frustrated percolation model of Coniglio *et al* [4], and other phenomenological models [5], however, different behaviours are obtained in other circumstances [1, 2, 6, 7].

Density relaxation can depend sensibly on many factors, such as geometry of grains, polydispersity, nature of friction forces, etc. As a simplified version of a granular system we consider a lattice of sites composed by a given number of horizontal layers in which sites may be occupied by the centre of identical particles. By taking the linear size of the particles greater than the lattice spacing excluded volume effects arise and relaxation can very likely be expected to be slower than exponential. We consider models for which friction and more complicated steric interactions are disregarded, so that the dynamics is

‖ E-mail address: mjoliveira@usp.br

¶ E-mail address: petri@unimo.it

0305-4470/98/220425+09$19.50 © 1998 IOP Publishing Ltd 

ruled only by inertial and excluded volume effects. Our aim is not to obtain a realistic model for granular compaction, but to study the relaxation process in circumstances that are simple enough to allow for an understanding of the dynamics of the process.

It has been observed that the compaction process which leads to maximum obtainable, random close packing, density is not reversible [2] and is obtained in the regime of low-energy perturbations. In contrast, energical shaking leads to states of lower density which appear to be reversible. Shaking or tapping at increasing energies involves large-scale collective motion of increasingly larger groups of grains, whereas low-intensity perturbations give rise to the motion of a few grains at a time, which in our model is represented by the diffusion of particles. In order to maintain dynamics at the simplest level we consider for the moment only horizontal (intra-layer) diffusion and downward movement. Particles diffuse along their own layer and owing to occasional fluctuations, regions of empty sites large enough to contain one more particle are created. If a particle of the neighbour upper plane is in correspondence with the newly created void it falls down, thus increasing the density of the lower layer and decreasing the density of the initial one. In a similar way a particle that, as a result of diffusion, finds itself upon a pre-existent void falls into the lower layer if the void is large enough to accept it.

In fact, in a real granular medium the final density depends on two more factors: (a) the way of preparation, i.e. the initial configuration and (b) the characteristics of the mechanical perturbation, for example, shaking or tapping amplitude and acceleration [1, 2]. A possible way of preparing the model under consideration is to fill the lattice layers in sequence from bottom to top. Initially one particle at a time is randomly placed in the bottom layer of the lattice without overlapping until no more particles can be placed in the plane. Then the upper nearest layer is filled according to the same rule, and so on for the others layers. This kind of preparation has the advantage of being well defined and statistically reproducible. In fact the process of placing sequentially nonoverlapping particles on lattices has been widely investigated in recent years. It is known as *random sequential adsorption* (RSA) [8] and has the remarkable property that the coverage so obtained is nonrandom in the thermodynamic limit. The present lattice model establishes a correspondence with the above-mentioned models and, moreover, it can be prepared in an initial state that, though stochastic in nature, possesses a well-defined and reproducible initial density $\rho$. This state is called a *jamming* state, and its density can in some cases be computed exactly [8]. In the past, assemblies of rigid squares and cubes have also been considered for studying some features of the liquid–solid transition [9, 10]. This allows for inferring more properties of the model that will be discussed elsewhere [11].

In order to carefully analyse the dynamical properties of the model and to see in which way slow relaxation behaviour is generated we proceed to specify the rules for the simplest system compatible with the above dynamics: we consider first a one-dimensional lattice with identical particles, said $k$-mers, each one occupying $k$ consecutive sites of the lattice. The particles do not overlap but can diffuse randomly with jumping rate $D$. The system is initially in the jamming state, i.e. no more particles can be added to the lattice before a rearrangement of the others. Subsequent diffusion gives rise to the formation of voids of size equal to or larger than $k$ lattice spacings, allowing for the introduction of other particles that we assume to occur through an ideal reservoir which places a new particle, at a deposition rate $R$, when at least $k$ consecutive empty sites are available. The resulting dynamics is related to the diffusional relaxation in RSA models [12]. When $R \to \infty$ we find the *diffusion-limited deposition* (DLD) model in which particles are added to the lattice as soon as required space is made available through diffusion. This situation also corresponds to taking the limit $D/R \to 0$.

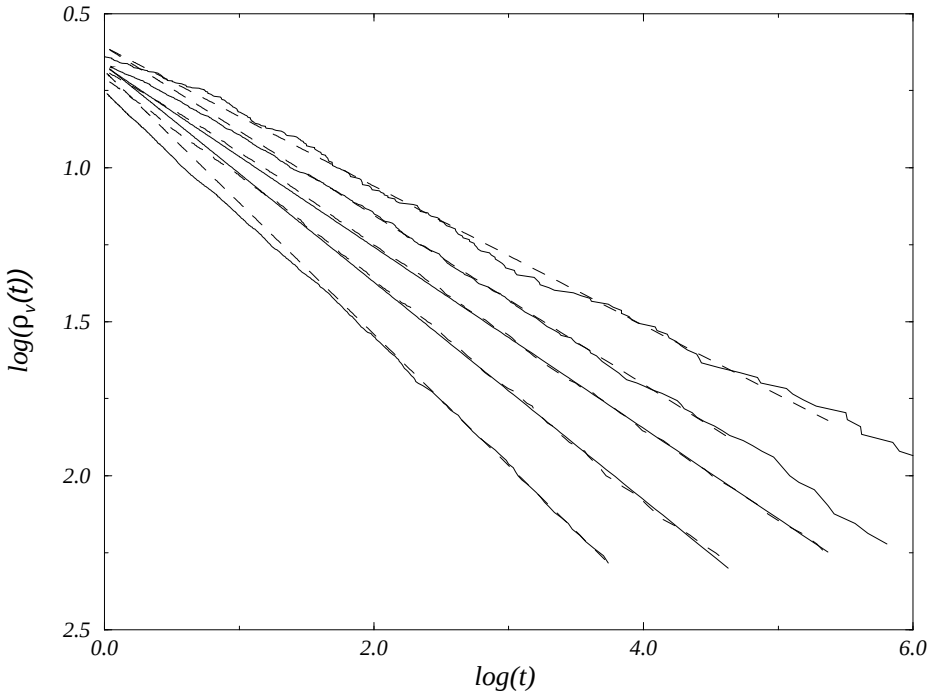


**Figure 1.** Numerically obtained values of $\rho_v(t)$ for the one-dimensional DLD of $k$-mers (averages over many realizations of 10 000 sites lattices). From left to right: $k = 3, 4, 5, 6, 8$. Resulting asymptotic exponents are reported in (4).

Temporal dependence of density in RSA models with diffusional relaxation has been investigated in the 1990s [12] and its expected behaviour can be derived by simple mean-field arguments. Instead of thinking of diffusing $k$-mers it is convenient to think in terms of diffusing vacancies, the locations of empty sites. In fact, in order to add a particle to the system it is necessary that $k$ vacancies meet themselves to form a $k$ *vacancy*. If we let $\rho_v$ be the fraction of vacant sites the above requirements yields

$$\frac{\mathrm{d}\rho_v}{\mathrm{d}t} \propto -\rho_v^k \tag{1}$$

from which it follows

$$\rho_v \sim t^{-\delta_k} \qquad \text{with } \delta_k = \frac{1}{k-1}. \tag{2}$$

The above result makes available one mechanism for the onset of a logarithmic behaviour. In fact, equation (2) implies that the algebraic relaxation becomes increasingly slower as $k$ increases, attaining a logarithmic behaviour in the $k \to \infty$ limit. This actually corresponds to considering a continuum system, with a vanishing lattice spacing $a$ such that $ak =$ constant. The limit can be carried out in different ways, bringing us to somewhat strictly different results [13], but in any case a logarithmic increase of density is found for such a one-dimensional system. For many systems the continuum limit is certainly of the most relevance, but a very important point is that, according to equation (2), a near logarithmic behaviour is attained in practice for any large $k$.

Asymptotic algebraic relaxation in DLD is very well reproduced by numerical simulations. However, exponents given by equation (2) are generally incorrect. In particular,

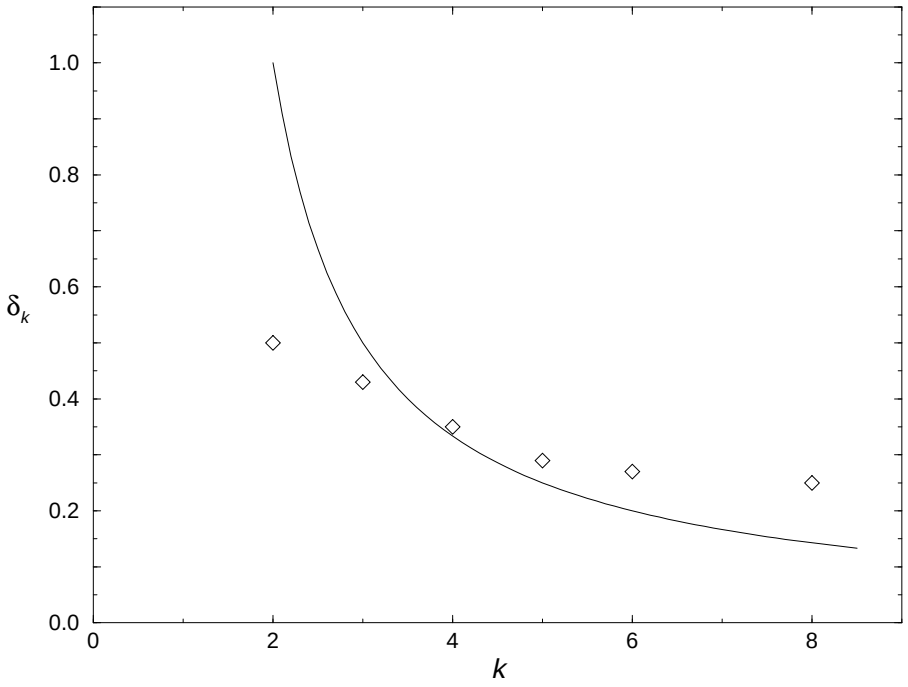


**Figure 2.** Exponent $\delta_k$ versus $k$ from mean field (curve) and simulations (diamonds).

in the case $k = 2$ it is well known that the exponent is $\frac{1}{2}$ [14], a sign that the process is governed by fluctuations of statistics rather than by averages. The correct exponent may in fact be obtained by considering that the time $t$ required by two diffusing vacancies to meet is proportional to the square of their relative distance $r$, and since $r \propto 1/\rho_v$, we find

$$\rho_v \sim t^{-1/2}. \tag{3}$$

Besides this argument the case $k = 2$ admits exact solutions in many different circumstances [15, 16], and several rigorous results have been established for the probability of two random walkers to meet in dimension from one [17] to three [18]. In contrast large-time behaviour for higher $k$ is not generally known. Moreover, numerical simulation for determining the annihilation rate of $k$ random walkers on a one-dimensional lattice display exponents that are generally different from mean-field ones but closer with those of a $k$-mer DLD†.

It has been argued that the mean field should work for $k \geqslant 4$ [14], this occurring for large enough times, namely $t \gg \exp(k)/k$. We have tried to test this hypothesis by performing numerical simulations of the $k$-mer DLD model for different values of $k$. Some numerical results are shown below together with the mean-field results

| $k$ | 2 | 3 | 4 | 5 | 6 | 8 |
|---|---|---|---|---|---|---|
| $\delta_k$ (mean field) | 1 | 0.50 | 0.33 | 0.25 | 0.20 | 0.14 |
| $\delta_k$ (numerical) | 0.50 | 0.40 | 0.35 | 0.29 | 0.27 | 0.25 |

(4)

and also in figures 1 and 2.

For $k < 4$ numeric exponents are lower than mean-field ones while for $k > 4$ they are higher, and are about the same for $k = 4$. To be reasonably certain of reaching an

† Numerical simulations of $k$ reaction walkers show exponents $\delta_k$ with small discrepancies from the present model, with the exception of the cases $k = 2$ and $k = 4$ when they are in agreement [19].

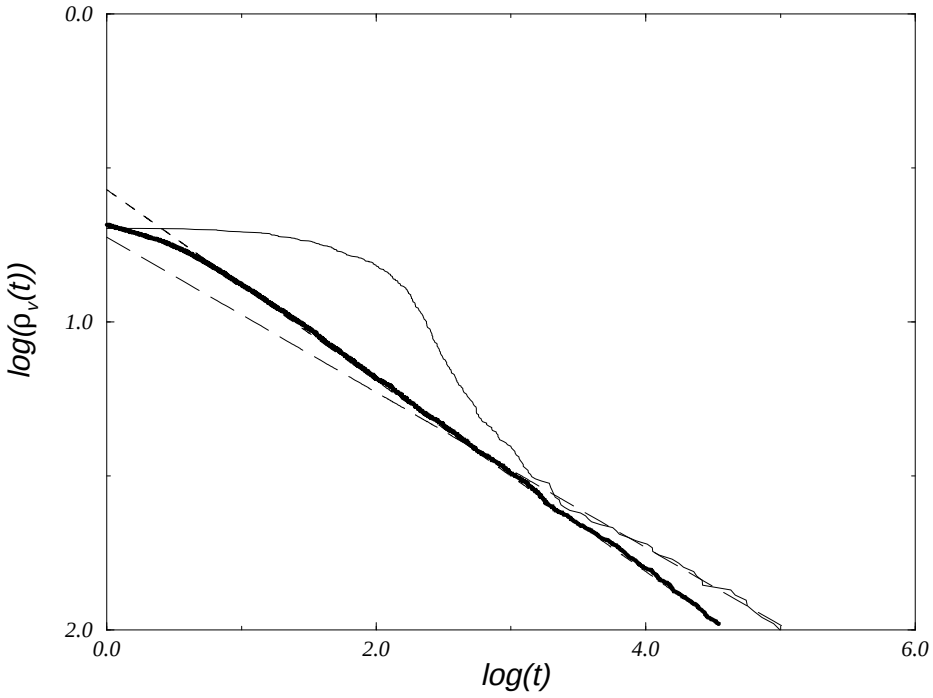


**Figure 3.** Decrease of vacancy density $\rho_v$ for DLD of pentamers on a lattice of $10^5$ sites (thick curve) and for the case $D/R = 999$ (thin curve). The exponent related to the latter case is the mean-field one. In fact from the simulation $\delta_5 = 0.25$ (the timescale of this curve has been left translated by $10^4$ units).

asymptotic regime in computer simulations it requires the use of wide systems and large computational time, thus it is not easy to say a definitive word on the validity of the mean-field figures. In any case figure 3 shows that the temporal decrease of $\rho_v$ down to values of about 0.01 for $k = 5$ in a lattice with $10^5$ sites does not exhibit any apparent deviation from the exponent in (4) (the simulation took more than 150 h of CPU time on a 466 MHz processor).

It has also been argued that the mean field should work at shorter times if the ratio $D/R$ is nonvanishing, since long-time diffusion without deposition may decorrelate the system. We did not observe such a behaviour for values of $D/R$ of about 10–100 on lattices of $10^5$ sites. However, simulation with $D/R \approx 1000$ also shown in figure 3, shows such a behaviour, suggesting that the mean-field regime had not yet been reached within the considered time for lower values of $D/R$. In other words, the smaller the value of $D/R$ the larger the time it takes to reach the mean-field behaviour. This statement implies that for $D/R = 0$ (DLD model) there will be no mean-field behaviour in agreement with the numerical result shown in (4).

Heretofore we have considered the case of just a single (one-dimensional) layer. In order to investigate the two-dimensional case let us start by studying the case of two- (one-dimensional) layers. We continue to consider that the upper layer obeys DLD, that is one more $k$-mer is added to it as soon as a $k$ vacancy is made available by diffusion. The rule is different for the lower layer where in order for a new $k$-mer to be added, not only a large enough void is necessary but, also, a $k$-mer must occupy the upper layer in exact

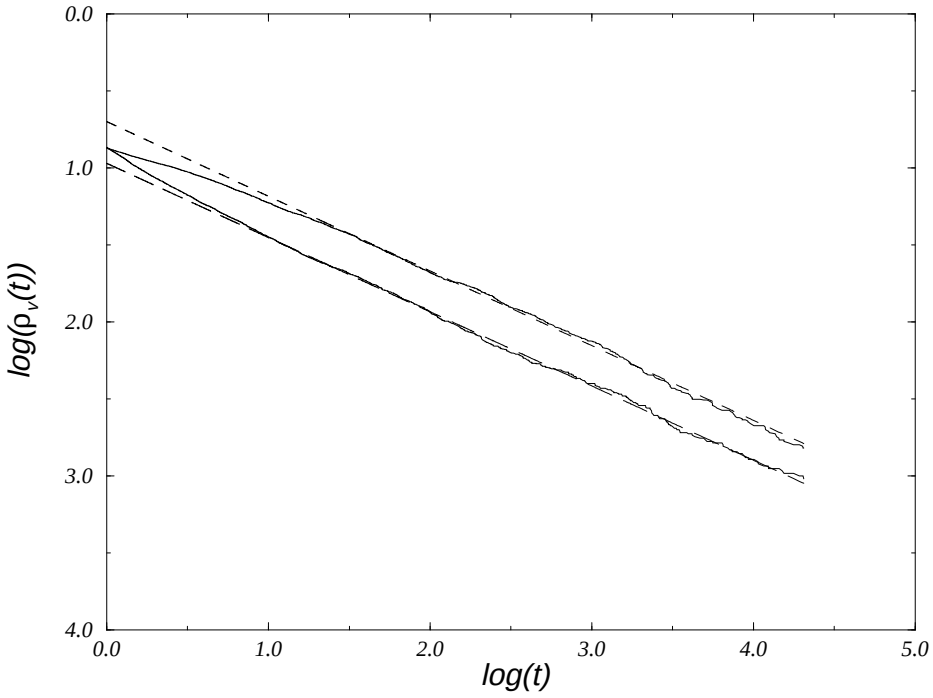


**Figure 4.** Dimer relaxation in a system made up of two layers of 50 000 sites each. The density of both layers increases with $\delta = 0.5$ as for a single layer.

correspondence with the $k$ vacancy. In principle this makes the dynamics in the lower layer very different, since $m$ vacancies with $m > k$ can be formed.

Let us consider, for instance, the case of dimers ($k = 2$). Using the same arguments as before we can compute mean-field exponents by considering the two possible processes that follow a diffusion. Process (a) corresponds to the formation of a di-vacancy in the lower layer, in correspondence with a dimer in the upper layer. Process (b) corresponds to a dimer in the upper layer that is displaced to occupy the sites which are upon a pre-existing di- or trivacancy (in fact no large vacancies are allowed with only two layers). If we let $\rho_1$ and $\rho_2$ be the densities of dimers respectively in lower and upper layers, the rates related to processes (a) and (b) are

$$R_a = \rho_1^2(1-\rho_1)^2\rho_2^2 \tag{5}$$

and

$$R_b = \rho_2^2(1-\rho_2)^2(1-\rho_1)^2 \tag{6}$$

respectively, leading to the time evolution equation for the density of the lower layer $\mathrm{d}\rho_1/\mathrm{d}t = R_a + R_b$. In the long-time limit, $\rho_1 \sim 1$ and $\rho_2 \sim 1$ so that

$$\frac{\mathrm{d}\rho_1}{\mathrm{d}t} = (1-\rho_1)^2 + (1-\rho_2)^2(1-\rho_1)^2. \tag{7}$$

The time evolution of the upper layer is independent of the lower layer and in the long-time limit is given by

$$\frac{\mathrm{d}\rho_2}{\mathrm{d}t} = (1-\rho_2)^2. \tag{8}$$

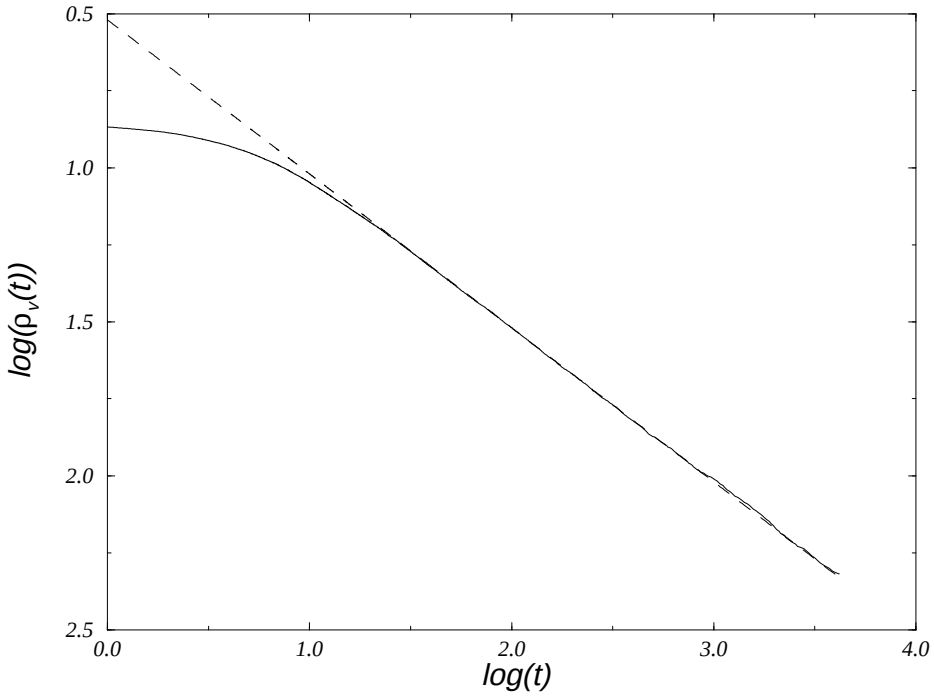


**Figure 5.** Dimer relaxation in more layers. A stationary phase at short time, owing to the presence of many layers, can be observed, after which the exponent approaches the same as that for one layer. Simulation was made by conserving the number of dimers.

Assuming algebraic dependence $1 - \rho_i \sim t^{-\alpha_i}$ one obtains to leading order in time $\alpha_i = 1$ for both $i = 1$ and 2, since dynamics is dominated by the process (a). This is the same mean-field exponent obtained in the case of a single layer. Since in the case of a single layer the mean field leads to an incorrect value we also expect it to happen in this case, even if it happens to be true that the two exponents are identical for the two layers. In fact, our numerical simulations show that $\alpha_i = \frac{1}{2}$ for both $i = 1$ and 2 (figure 4). The dominance of process (a) in the long-time limit, which leads to the identity of the two exponents, is an indication that the upper layer works like a reservoir of particles for the lower layer.

We do not write down more complicated equations for increasing numbers of layers, and proceed directly to discuss the numerical results. We simulated systems of dimers up to 10 000 sites $\times$ 100 layers. We observed that the density of each single layer fluctuates more when compared with the case of only a few layers. Moreover, a delay between the initial time and the time at which a sensible increase of density start to appear arises. This delay becomes increasingly larger as the number of layers is increased, giving rise to an overall initial slowing in the density change, as shown in figure 5, a fact that could be relevant to the understanding of the logarithmic behaviour also observed at short times in many systems [2–5]. However, no change is observed in the large-time dependence of the total density. We have also checked the influence of the top boundary condition by imposing conservation of the number of particles, i.e. by removing the reservoir on the top. In this case a few of the upper layers of the lattice emptied during the process, but we could not observe any change in the total density behaviour.

We obtained the same results by simulating systems made by trimers, so we expect

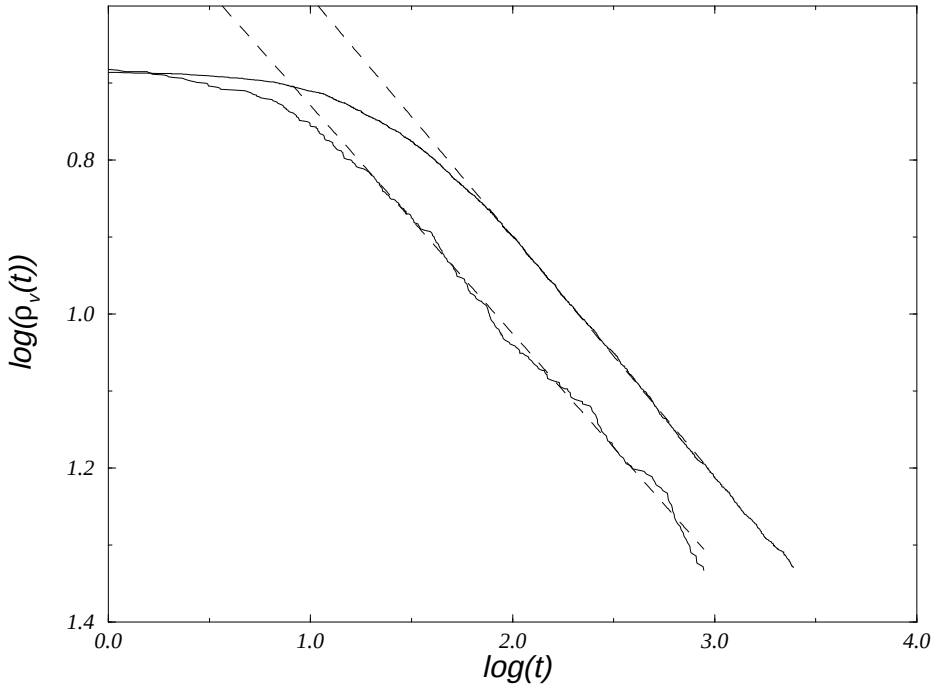


**Figure 6.** Relaxation of a conserved number of pentamers in two lattices of different sizes. The exponents found are consistent with that of a single layer ($\delta = 0.30$, $\delta = 0.31$).

the exponent also not to change for $k = 4$. However, the behaviour in one dimension for $k > 4$ suggested that we investigate the case $k = 5$. In fact the interaction among different layers is such that diffusion may occur for a very long time before a vacancy succeeds in being filled, thus creating a situation similar to the case $D/R \gg 1$ discussed above in one dimension. The numerical effort required in this case is much larger than in the one-dimensional case. Here we report the result from a lattice made by 2000 sites $\times$ 20 layers and another made by 4000 sites $\times$ 100 layers (see figure 6); as a consequence of the large time required, the two simulations stop at different times and densities. However, they seem to indicate that the same exponent as in the one-dimensional case with $R \to \infty$ still holds (cf the different behaviour in figure 3). This point is of some relevance because validity of mean-field exponents would lead to $\delta \to 0$ (consistent with a logarithmic behaviour) in the continuum limit. In the opposite case a different result for $k \to \infty$ cannot be excluded. Finally we wish to remark that other behaviours than those discussed here can be obtained by adopting different rules for the proposed lattice model [11].

We are grateful to Vittorio Loreto for many stimulation and clarifying discussions. This work was supported by a grant from Laboratório de Computação Avançada of the Universidade de São Paulo (LCCA-USP) and by a grant from Universidade de São Paulo.

## References

[1] Jaeger H M, Nagel S R and Behringer R P 1996 *Rev. Mod. Phys.* **68** 1259
[2] Knight J B, Fandrich C G, Lau C N, Jaeger H M and Nagel S R 1995 *Phys. Rev.* E **51** 3957
[3] Caglioti E, Loreto V and Herrmann H J 1997 *Phys. Rev. Lett.* **79** 1575

[4] Coniglio A and Herrmann H J 1996 *Physica* **225A** 1
[5] Linz S J 1996 *Phys. Rev.* E **54** 2925
[6] Barker G C and Metha A 1993 *Phys. Rev.* E **47** 184
[7] Hong D C, Yue S, Rudra J K, Choi M Y and Kim Y W 1994 *Phys. Rev.* E **50** 4123
[8] Evans J V 1993 *Rev. Mod. Phys.* **65** 1281
[9] Zwanzig R W 1956 *J. Chem. Phys.* **24** 855
[10] Gount D S and Fisher M E 1965 *J. Chem. Phys.* **43** 2840
[11] Loreto V, de Oliveira M J and Petri A to be published
[12] Privman V, Wang J-S and Nielaba P 1991 *Phys. Rev.* B **43** 3366
Bartelt M C and Privman V 1991 *Int. J. Mod. Phys.* B **5** 2283
[13] Privman V and Barma M 1992 *J. Chem. Phys.* **97** 6714
[14] Nielaba P and Privman V 1992 *Mod. Phys. Lett.* B **6** 533
[15] Eisberg E and Baram A 1997 *J. Phys. A: Math. Gen.* **30** L271 and references therein
[16] Barma M, Grynberg M D and Stinchcombe R B 1993 *Phys. Rev. Lett.* **70** 1033
[17] Fisher M E 1985 *Fundamental Problems in Statistical Mechanics* ed E G D Cohen (Amsterdam: Elsiever)
[18] Bramson M and Lebowitz J C 1988 *Phys. Rev. Lett.* **61** 2397
[19] de Oliveira M J and Petri A to be published
[20] Privman V and Gryndberg M D 1992 *J. Phys. A: Math. Gen.* **25** 6567