Granular Matter 3, 57–61 © Springer-Verlag 2001

Glassy models for granular systems

Jeferson J. Arenzon, Mauro Sellitto

Abstract We briefly review some simple lattice models, introduced recently to study granular systems based on the similarities with glassy systems. The basic common ingredient, partially responsible for the complex behavior shown, is geometric frustration due to steric hindrance.

Keywords Granular matter, glassyness, lattice models

1 Introduction

For many agricultural and industrial processes, proper handling of granular material pose several fundamental practical problems that only recently have attracted the attention of physicists [1–3]. Because of its unusual static and flowing properties, the subject offers a challenging problem from the theoretical point of view, and despite the huge effort devoted to them, are far from being fully understood. Therefore, since even the basic mechanisms responsible for the very unintuitive properties presented by these systems are still matter of debate, simple lattice models have been recently introduced in order to clarify these issues as well as to provide a framework where analytical treatment may be more feasible.

Granulars also provide one of the most interesting examples of macroscopic out-of-equilibrium behavior and may serve as an easy setup, experimental test bed. In particular, since they share several properties with glasses, some of the properties (like fluctuation-dissipation violations) may be more accessible to test here. Due to the size of the grains, thermal energy plays no role and although the system may be easily trapped in one of the many existing metastable states, excitations can be achieved by externally shaking or shearing the system, enabling it to wander through the many microscopic configurations available for fixed macroscopic parameters. Under vibration, a multitude of fascinating phenomena show up, (see [1–3] for a review and references), being compaction, aging and segregation the ones that concern us here most [4].

Slow relaxation under perturbation, signalling complex cooperative movements of the particles, is readily seen in compaction experiments [5]. Interestingly, other systems where the dynamics is ruled by the presence of a multitude of metastable states, like structural glasses and spin glasses, indeed behave in a similar fashion. For the granulars, the increase in the bulk density as the system is either shaken or tapped follows an inverse logarithm law

$$\rho(t) = \rho_\infty - \frac{\Delta\rho_\infty}{1 + B \ln(1 + t/\tau)}, \tag{1}$$

with several fit parameters that depend on the vibration amplitude. This behavior is well supported by experimental results [5], numerical simulations [6–9], and analytical approaches [11–16] essentially based on free-volume models familiar from the physics of glasses. Related to slow relaxation, these systems present aging properties [17,18]. While one-time quantities asymptotically tend to their equilibrium values, two-times quantities depend explicitly both on the observation time and on the time elapsed since the perturbation was applied: time translation invariance (TTI) is broken, which is a manifestation of history dependence, that is, the system ages. Moreover, fluctuation-dissipation relations no longer hold when in the out-of-equilibrium regime, although analytical and numerical evidence from the study of some model glasses point to a generalization of it [19]. Although these properties have been studied at length for spin and structural glasses, only recently, as the glassy nature of granular systems became clear, similar properties start being reported in such a systems.

Another puzzling behavior presented by granular materials is size segregation, where a mixture of particles of different sizes get separated under vibrations, the larger particles raising to the top. This phenomenum is easily noticed in several different experimental setups like, for instance, rotating drums, vertical and horizontal shaking or simply by pouring the powder onto a pile. Several distinct mechanisms may play a role (see [20–24] and also [1–3,25]).

The objective of this paper is briefly review and compare some of the simple lattice models recently introduced in the study of powders, along with their glassy counterparts, where the system is not externally driven by gravity. Several equilibrium and out-of-equilibrium properties

Received: 30 March 2000

J. J. Arenzon (✉)
Instituto de Física
Universidade Federal do Rio Grande do Sul
91501-970 Porto Alegre RS – Brazil
e-mail: arenzon@if.ufrgs.br

M. Sellitto
Laboratoire de Physique de l'École
Normale Supérieure de Lyon
46 Allée d'Italie, 69007 Lyon – France
e-mail: mauro.sellitto@enslapp.ens-lyon.fr

Work partially supported by the brazilian agency CNPq.

are described, highlighting both the similarities and differences between thesem systems.

2
Lattice models for glassy and granular systems

Although several simple models have been proposed to explain logarithmic compaction and segregation, we will review and compare only some lattice models, based on the geometric frustration concept, that make the connection with some features of the glassy physics. In $2d$, the system is defined on a 45°-tilted lattice: there is no movements along the horizontal, particles can only go up or down. In $3d$, this can be easily achieved by considering a bcc lattice. We may write these models in the form

$$\mathscr{H} = -J \sum_{\langle ij \rangle} f_{ij}(S_i, S_j) n_i n_j - g \sum_i n_i h_i \tag{2}$$

where $n_i = 0, 1$ ($i = 1 \dots N$) are local densities or site occupations and there is a frustration term f_{ij} that depends on the internal degrees of freedom (e.g. rotational ones). Although molecules in glass forming liquids or particles in granular systems may assume several spatial orientations, here we take the simpler cases of either no such degrees of freedom (constant f_{ij}) or only two possibilities, $S_i = \pm 1$. The models that will be considered are the Frustrated Ising Lattice Gas (FILG) [30,31] with

$$f_{ij} = \varepsilon_{ij} S_i S_j - 1 \tag{3}$$

where $\varepsilon_{ij} = \pm 1$ are quenched random variables, the Tetris [7] with

$$f_{ij} = \frac{1}{2} \left[S_i S_j - \varepsilon_{ij} (S_i + S_j) + 1 \right] \tag{4}$$

where, differently from the FILG, the bonds ε_{ij} are not random, but $+1$ along one diagonal and -1 along the other, and the Kob-Andersen [9,27] one with

$$f_{ij} = 0 \ . \tag{5}$$

While the FILG is purely Hamiltonian, the Tetris model has a further kinetic rule for updating the internal degrees of freedom depending on the local densities. The Kob-Andersen, on the other hand, is purely kinetic. In any case, the physical basis for both the kinetic constraints and the frustration terms is the usually complex spatial structure of the particles (either grains or molecules) that is in part responsible for the geometric constraints, imposed by the neighbors, on their translational and rotational dynamics.

2.1
The Frustrated Ising Lattice Gas

Without gravity, both the equilibrium [33,34] and the out-of-equilibrium [35–37] properties have been studied for $T = 1$ and $J = 10$, corresponding to the Frustrated Percolation limit (where $J \to \infty$) [30,31]. In this limit, in order to minimize $\mathscr{H}$, Eqs. (2–3), either the spins should satisfy the bond ε_{ij} or at least one of the sites i or j must be empty. Moreover, the condition of large J may be relaxed or a dynamics can be implemented for the bonds ε_{ij} [32].

In the low density regime the behavior is liquid like, time correlation functions decay exponentially, equilibration is quickly achieved and the particles mean squared displacement grows linearly with time, a simple diffusion scenario since particles hardly feel any constraint in their mobility. At a higher density, there is a percolation transition, that manifests dynamically as a first, fast exponential relaxation at short times and as a slow, stretched exponential relaxation at longer ones. At a density $\rho_c \simeq 0.67$, the relaxation times diverge and the diffusion constant goes to zero, transition that corresponds to the dynamical one in mean field p-spin or Potts glasses or the ideal glass transition in the mode coupling theory. Also, the spin glass susceptibility, associated with the internal degrees of freedom of occupied sites, diverges at the same point where a glass transition takes place [33,34], signalling a thermodynamic spin glass transition associated with the frozen-in of the internal degrees of freedom.

A characteristic feature of out of equilibrium glassy systems is slow aging dynamics [17,18], present in the FILG both with [42] and without gravity [35]. The decay of autocorrelations is similar to that observed in molecular dynamics simulations of Lennard-Jones glasses. A typical aging scenario is present signalling the slowing down of the dynamics as the waiting time from the application of the perturbation grows. For long waiting times, the correlation presents a rather fast relaxation to a plateau in which the system evolves in quasi-equilibrium: the dynamics is stationary and the fluctuation-dissipation relations hold. The plateau separates two time scales typical of glassy systems: a β (fast) relaxation for short times and an α (slow) relaxation at longer times, corresponding respectively to the fast movements of the particles inside the dynamical cages and the large scale, cooperative process that takes much more time in order to rearrange the cages. Moreover, in this long time regime, the system falls out of equilibrium, the correlations decay to zero asymptotically and time translational invariance (TTI) no longer holds with the corresponding violation of the fluctuation-dissipation theorem (FDT). An analogous aging scenario has been found in presence of gravity [42], although the scaling of the correlation functions is somewhat different. In the out-of-equilibrium regime, where FDT is violated, there are, on the other hand, evidences from simulation and mean field calculations, that a generalized relation between two times correlation functions $C(t, t_w)$ and the associated responses $R(t, t_w)$ still holds [17,18], involving a "Fluctuation-Dissipation Ratio" (FDR), connected to an effective temperature. Interestingly, the form of the FDT violation, shown by the FILG without gravity, is exactly the one predicted in these mean field models considered as good models for glasses, i.e. a constant FDR, signalling that this model presents two very separated time scales [36]. Moreover, this may be the first realization of a glassy phase characterized by one step of replica symmetry breaking (in the Parisi scheme) in a finite dimensional model. When gravity is included, the form of the FDT violation is much more complicated, as will be shown in the next session for the Tetris model, and reported to be similar in the FILG [45].

Another similarity between the glassy and granular cases appears when a sort of cooling experiments are performed. In the case of glasses, by decreasing the temperature at a given rate, below the melting point, liquids may either crystallize or enter a supercooled regime. As

the glass transition temperature T_g is approached, molecular motion gets slower and slower and relaxation times increase by several orders of magnitude and for all practical purposes the system remains out of equilibrium. This transition temperature T_g is rate dependent and is still matter of debate if there is an underlying thermodynamical transition. This scenario is exactly what happens in the FILG [37] when changing the chemical potential at different rates: for each compressing rate, the system goes out of equilibrium at different points. With gravity, by varying the vibration amplitude, the system presents reversible-irreversible cycles [38]: after pouring the particles and performing low amplitude vibrations, the density increases as the system escapes from the initial, low density metastable states. Further increasing the amplitude, at a certain point, decompactification starts and the density diminishes after passing the maximum. By reverting the cycle, decreasing the amplitude, the curve follows the previous one up to a given point, departing from it and forming the reversible part of the cycle. The actual paths are rate dependent: the system goes out of equilibrium at different points for different rates. This sequence of paths is quite well reproduced by the FILG model [42].

At a mean field level, equilibrium properties have been studied in closely related models with [39] and without gravity [40,41]. When all sites are occupied, the behavior corresponds to the Sherrington-Kirkpatrick model, with a continuous spin glass transition. Upon decreasing the density, one reaches a tricritical point, below which the transition is first order. In this region, analogously to other first order transition models like the p-spin and the Potts glass, above the critical temperature there is a dynamical transition where metastable states first appear. We still do not know in what extension this scenario remains valid in finite dimensions, but the results from the study of the violation of the fluctuation-dissipation theorem indicates [36] a high similarity between the $3d$ model and mean-field models with a discontinuous transition (and one step of replica symmetry breaking). By including gravity, depending on the amount of vibration, the system suffers a fluidization transition: the upper part of the system may be in a liquid-like phase while the bottom one is in solid-like one. As the vibration increases, the layer separating both regimes approaches the bottom of the system and above a critical temperature, all layers are liquid-like. Although interesting, the mean field version of the model has still to be tested to whether or not it presents slow compaction (since the number of connections to satisfy increases in the mean field limit, we do expect slow behavior, not necessarily the same as in finite dimensions).

2.2 The Tetris model

In analogy with the computer game "Tetris", where blocks of a myriad of forms fall and must be arranged in such a way to avoid vacancies, here, non-overlapping, elongated grains try to arrange in an alternate (anti-ferromagnetic) ordering [7,43]. The model, apart being described by Eqs. (2–4), has a kinetic constraint for possible changes of orientation of particles, depending on local densities: in not too dense regions, particles may rotate.

Although the compaction again follows the inverse logarithm law, Eq. (1), there are some differences in the underlying mechanism when compared with the FILG [44], the growth of the largest cluster being different in both cases.

Response functions, and the relation with the characteristic fluctuations (the so called "Fluctuation-Dissipation Relation") have been extensively studied in the Tetris model [45,8]. Two replicas of the system are compared during the dynamical evolution where, at a time t_w the vibration amplitude of one of them is slightly changed. The difference in the height of the center of mass in both replicas, $\Delta h(t, t_w)$, is related to the mean square displacement $B(t, t_w) = \langle [h(t) - h(t_w)]^2 \rangle$ in the unperturbed system. By being externally driven, the system presents spatial heterogeneities (for instance, between bulk and interface) that are different from the FILG without gravity and should be carefully taken into account, as shown by Barrat and Loreto [8]. Responses may be either positive or negative, depending on the degree of compaction of the perturbed system when compared with the unperturbed one. The response has an initial positive branch and, for larger times (that depends on both the waiting time and the vibration amplitude), a negative one. The positive part gets larger as t_w increases, signalling that the system history and how it is driven are important ingredients when trying to define an effective temperature based on generalized fluctuation-dissipation relations.

Grains of different forms may also be introduced, generalizing the model [43,8], to test for segregation. The particle separation is directly related to the presence of different mobilities, allowing for the sifting of the small particles. An analogous mechanism for segregation is also present in the Kob-Andersen model, as will be shown in the next section.

2.3 The Kob-Andersen model

Kob and Andersen [27] used a kinetically constrained lattice-gas made of non interacting, non overlapping particles to model the properties of supercooled liquids. In this way, the model is purely kinetic ($\mathscr{H} = 0$), the rule mimicking the effect of steric hindrance present in real glasses: one randomly chosen particle may hop to an empty neighboring site if before and after the movement the particle has less than ν other nearest neighbor particles. By construction, every initial state is an equilibrium state of the system and no further equilibration is needed (TTI and FDT relations are obbeyied). Nevertheless, by letting the system exchange particles with a reservoir (for example, in the outermost layers), it is possible (similarly to a compression) to observe the off equilibrium dynamics of the system [28,29]. In this way, the main features of glassy physics are well reproduced by this very simple model. In particular, in the equilibrium regime, as the density increases, particles movements become more constrained and are only allowed after a large, cooperative rearrangement of the neighboring particles. The associated cooperative length increases with the system density and at a

threshold density, $\rho_c \simeq 0.88$, the diffusion coefficient goes to zero, signalling a glass transition. This effect is purely dynamical since the lack of interaction implies a trivial thermodynamics: no thermodynamical transition exists for this model.

The Kob-Andersen can model granular systems by taking into account gravity [9,10], Eqs. (2–5) and $\nu = 5$. From the static point of view, there is only a lattice-gas of non-interacting particles in a gravity field and, again, the thermodynamics is trivial and it is only because of the kinetic constraint that there is an interesting behavior, in accordance with the basic granular phenomenology. Indeed, gravity and weak vibrations combined produce, as in previous models, a slow increase in the packing density of the system, according to the inverse logarithmic law, Eq. (1). However, for strong vibrations, although the above law still provides a reasonable description of the compaction process for the whole time window, a modified version (but still logarithmic) or a power law (for large times) also provide a consistent, sometimes better, fit [10]. From these fits, the asymptotic packing density seems to depend on the vibration amplitude. For very high amplitudes, the decompactification achieved by the system is enough to decrease the density such that the constraints are no longer important (the condition on the number of neighbors is hardly needed). In this regime, the behavior is in accordance with the thermodynamical picture: the packing density is a decreasing function of the vibration amplitude. Lowering the vibration, the constraints become important and there is a dynamical jamming transition. In the other extreme, for small amplitude vibrations, the system is trapped in one of the many low density metastable states, being unable to explore denser neighbor configurations, and any further increase in the vibration helps the system to increase its density. In between, there is an optimal value of the vibration amplitude for which the asymptotic density is maximum.

Moreover, a polydisperse system of particles, with different degrees of kinetic constraints (yet identical masses), can be considered in order to show that segregation phenomena is present in the Kob-Andersen model. Both components differ only in the value of ν in the kinetic constraint: one type of particle is constrained while the other one is not. Starting from a random homogeneous distribution of particles, under vibration, the constrained (large) particles rise to the interface region, while the unconstrained (small) ones sift to the bottom. The mechanism is analogous to the one present in the Tetris model [43]: small particles, because of their greater mobility, easily fill the gaps beneath large ones.

Although the model is still in early stages of research, in analogy with the $g = 0$ version, we expect that other properties (e.g., response functions and the corresponding correlation functions, reversible-irreversible cycles, etc) will be well reproduced.

3 Conclusions

We discussed simple lattice models whose common key ingredient is a free-volume constraint, implemented in several ways, to mimic geometric frustration effects. The models discussed here may be divided in three categories: some are fully kinetical, some are purely Hamiltonian while others are a mixing of both. Although the objective is not to provide a realistic, quantitative description, the basic granular phenomenology is quite well reproduced by these models, showing the robustness of the phenomena in spite of details of the microscopic models. Indeed, from the experimental point of view, granular systems present a rather universal behavior, irrespective of the details of the grains. Moreover, these models, without gravity, are quite successful in describing glassy properties, clarifying the relation among these two systems, apparently so different. In particular, for the Kob-Andersen model, this similarity is obtained without introducing any form of quenched randomness neither in the energetic interaction nor in the shape of particles.

In a nutshell, simple lattice models are able to capture the main dynamical properties of systems where geometric frustration is a dominant mechanism responsible for slow relaxation, unifying, in this way, rather different systems, granular and glassy.

References

1. H. M. Jaeger, S. R. Nagel, & R. P. Behringer, Granular solids, liquids, and gases, Rev. Mod. Phys., 68 (1996), p. 1259–1273
2. P.-G. de Gennes, Reflections on the mechanics of granular matter, Physica A 261 (1998), p. 267–293
3. L. P. Kadanoff, Built upon sand: Theoretical ideas inspired by granular flows, Rev. Mod. Phys., 71 (1999), p. 435–444
4. For static properties, see the contribution of C. Moukarzel in this volume
5. J. B. Knight, C. G. Fandrich, C. N. Lau, H. M. Jaeger, & S. R. Nagel, Density relaxation in a vibrated granular material, Phys. Rev. E 51 (1995), p. 3957–3962
6. A. Coniglio & H. J. Herrmann, A model for the compaction of granular media, Physica A 225 (1995), p. 1–6
7. E. Caglioti, V. Loreto, H. J. Herrmann, & M. Nicodemi, A "Tetris-like" Model for the Compaction of Dry Granular Media, Phys. Rev. Lett. 79 (1997), p. 1575–1578
8. A. Barrat & V. Loreto, Response properties in a model for granular matter, J. Phys. A 33 (2000), 4401
9. M. Sellitto & J. J. Arenzon, Free-volume kinetic models of granular matter, Phys. Rev. E 62 (2000), 7793
10. J. J. Arenzon & M. Sellitto, (2000)
11. T. Boutreux & P.-G. de Gennes, Compaction of granular mixtures: a free volume model, Physica A 44 (1997), p. 59–67
12. E. Ben-Naim, J. B. Knight, E. R. Nowak, H. M. Jaeger, & S. R. Nagel, Slow relaxation in granular compaction, Physica D 123 (1998), p. 380–385
13. K. L. Gavrilov, Cluster model for compaction of vibrated granular materials, Phys. Rev. E 58 (1998), p. 2107–2114
14. D. A. Head & G. J. Rodgers, A coarse-grained model for granular compaction and relaxation, J. Phys. A 31 (1998), p. 107–122
15. D. A. Head, A phenomenological glass model for vibratory granular compaction, Phys. Rev. E 62 (2000), 2439
16. J. J. Brey, A. Prados, & B. Sánchez-Rey, Simple model with facilitated dynamics for granular compaction, Phys. Rev. E 60 (1999), p. 5685–5692

17. J. P. Bouchaud, L. F. Cugliandolo, J. Kurchan, & M. Mézard, in Spin Glasses and Random Fields, Ed. A. P. Young (World Scientific, Singapore, 1998)
18. E. Vincent, J. Hammann, M. Ocio, J. P. Bouchaud, & L. F. Cugliandolo, in Proceedings of the Sitges Conference on Glassy Dynamics, Ed. E. Rubi (Springer, Berlin, 1996)
19. L. F. Cugliandolo & J. Kurchan, Analytical Solution of the Off-Equilibrium Dynamics of a Long-Range Spin-Glass Model, Phys. Rev. Lett. 71 (1993), p. 173–176
20. J. C. Williams, The Segregation of Particulate Materials: A Review, Powder Technol. 15 (1976), p. 245
21. A. Rosato, K. J. Strandburg, F. Prinz, & R. H. Swendsen, Why the Brazil nuts are on top: Size segregation of particulate matter by shaking, Phys. Rev. Lett. 58 (1987), p. 1038–1040
22. J. B. Knight, H. M. Jaeger, & S. R. Nagel, Vibration-induced size separation in granular media: The convection connection, Phys. Rev. Lett. 70 (1993), p. 3728–3731
23. T. Shinbrot & F. J. Muzzio, Reverse Buoyancy in Shaken Granular Beds, Phys. Rev. Lett. 81 (1998), p. 4365–4368
24. H. A. Makse, S. Havlin, P. R. King, & H. E. Stanley, Spontaneous stratification in granular mixtures, Nature 386 (1997), p. 379–382
25. See also the contribution of R. Monetti, A. Hurd & V. M. Kenkre, in this volume, for an application of a related simple model [26] in the problem of horizontal segregation in rotating drums
26. S. Katz, J. L. Lebowitz, & H. Spohn, Phase transitions in stationary nonequilibrium states of model lattice systems, Phys. Rev. B 28 (1983), p. 1655–1658
27. W. Kob & H. C. Andersen, Kinetic lattice-gas model of cage effects in high-density liquids and a test of mode-coupling theory of the ideal-glass transition, Phys. Rev. E 48 (1993), p. 4364–4377
28. J. Kurchan, L. Peliti, & M. Sellitto, Aging in lattice-gas models with constrained dynamics, Europhys. Lett. 39 (1997), p. 365–370
29. L. Peliti & M. Sellitto, Aging in a simple model of a structural glass, J. Physique
30. A. Coniglio, Frustrated Percolation, Spin Glasses and Glasses, Nuovo Cimentof D 16 (1994), p. 1027–1037
31. A. Coniglio, Spin glasses, glasses and granular materials, Phil. Mag. B 77 (1998), p. 213–219
32. A. Fierro, Glassy dynamics in systems with quenched and annealed interactions, Ph.D. thesis, Università di Napoli, Naples, Italy (2000)
33. M. Nicodemi & A. Coniglio, The glassy transition of the frustrated Ising lattice gas, J. Phys. A 30 (1997), p. L187–L194
34. M. Nicodemi & A. Coniglio, Macroscopic glassy relaxations and microscopic motions in a frustrated lattice gas, Phys. Rev. E 57 (1998), R39–R42
35. D. Stariolo & J. J. Arenzon, Off-equilibrium dynamics of the frustrated Ising lattice gas, Phys. Rev. E 59 (1999), p. R4762–R4765
36. F. Ricci-Tersenghi, D. Stariolo, & J. J. Arenzon, Two-times scales and FDT violation in a Finite Dimensional Model for Structural Glasses, Phys. Rev. Lett. (2000) in press
37. J. J. Arenzon, F. Ricci-Tersenghi, & D. Stariolo, Aging dynamics of the Frustrated Ising Lattice gas, Phys. Rev. E 62 (2000) 5978
38. E. R. Nowak, J. B. Knight, M. Povinelli, H. M. Jaeger, & S. R. Nagel, Reversibility and irreversibility in the packing of vibrated granular material, Powder Technol. 94 (1997), p. 79–83
39. J. J. Arenzon, Replica theory of granular media, J. Phys. A 32 (1999), p. L107–L113
40. J. J. Arenzon, M. Nicodemi, & M. Sellitto, Equilibrium Properties of the Ising Frustrated Lattice Gas, J. de Physique 6 (1996), 1143–1152
41. M. Sellitto, M. Nicodemi, & J. J. Arenzon, The Blume-Emery-Griffiths Spin Glass Model, J. de Physique 7 (1997), p. 945–957
42. M. Nicodemi & A. Coniglio, Aging in Out-of-Equilibrium Dynamics of Models for Granular Media, Phys. Rev. Lett. 82 (1999), p. 916–919
43. E. Caglioti, A. Coniglio, H. J. Herrmann, V. Loreto, & M. Nicodemi, Segregation of granular mixtures in the presence of compaction, Europhys. Lett. 43 (1998), p. 591–597
44. M. Nicodemi, Domain growth and packing properties in driven granular media subject to gravity, (1999), preprint, `cond-mat/9911338`
45. M. Nicodemi, Dynamical Response Functions in Models of Vibrated Granular Media, Phys. Rev. Lett. 82 (1999), p. 3734–3737