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# The frustrated lattice gas: a microscopic model for the glass transition

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**Abstract**

The out-of-equilibrium behavior of the frustrated lattice gas, a model of structural glasses, is described, showing many of the essential features of glass phenomenology. The relation with well-known spin glass models may help in understanding many controversial issues related with the liquid–glass transition and glassy dynamics of many physical systems. © 2000 Elsevier Science B.V. All rights reserved.

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Many theoretical aspects of the structural glass transition and the nature of the glassy phase (see e.g. the articles in Ref. [1]) are still poorly understood and as the involved physics gets more and more complex, the lack of a tractable microscopic model is felt. Little, analytical progress has been made with popular models based on Lennard–Jones potentials which, on the other hand, have been extensively studied via molecular dynamics simulations [2]. Meanwhile, in the field of spin glasses, disordered magnetic systems which share many physical properties with structural glasses, a reasonable theoretical understanding of the basic physics has been achieved at least at the mean field level [3,4]. Recently, it has been found that the equations describing dynamic correlations and response functions of a kind of mean field spin glasses above the transition temperature are formally the same as those found in the mode coupling theory of supercooled liquids [5]. This points to a deeper analogy between the physics of spin glasses and structural glasses than previously thought. Nevertheless, up to now we do not know to which extent this analogy can be pushed forward. Some important

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differences between these two kinds of systems are evident: while a defining feature of spin glasses is the quenched disorder and frustration, no such quench disorder is evident in structural glasses. Another important difference is the fact that the dynamical variables in a spin glass are localized in space and do not diffuse as the molecules in a supercooled liquid. We would like to have at hand a simple, yet non trivial microscopic model of supercooled liquids in which we could apply the fruitful techniques developed in spin glass theory.

A possible such model is the frustrated lattice gas introduced some years ago [6,7]. The model, in a $d$-dimensional lattice, is defined by the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} (\varepsilon_{ij}\sigma_i\sigma_j - 1)n_i n_j - \mu \sum_i n_i \,. \tag{1}$$

There are two kinds of dynamical variables: the local density or occupation $n_i = 0, 1$ ($i=1,\ldots,N$) and the particles internal degrees of freedom, $\sigma_i=\pm 1$. The usually complex spatial structure of the molecules in glass forming liquids, which can assume several spatial orientations (here we take the simplest case of only two orientations), is in part responsible for the geometric constraints, imposed by the neighbors, on their dynamics. This hindrance effect is encapsulated in the quenched random variables $\varepsilon_{ij} = \pm 1$. The key role of the first term of the Hamiltonian is that when $J \to \infty$ the (site) Frustrated Percolation [6,7] is recovered, where no frustrated link can be fully occupied, implying that any frustrated loop in the lattice will have a hole and then $\rho < 1$, preventing the system from reaching the close packed configuration. Finally, $\mu$ represents a chemical potential ruling the system density (at fixed volume) and, by taking $\mu \to \infty$ while keeping $J$ finite, we recover the well-known Edwards–Anderson spin glass model.

The equilibrium properties of the model have been numerically studied by Nicodemi et al. [8,9]. A spin glass susceptibility, associated with the internal degrees of freedom, has been found to diverge at $\mu \simeq 5.5$, corresponding to a density $\rho \simeq 0.67$. Meanwhile, the compressibility associated with the density variables does not present critical behavior but only a maximum as observed in many glass-formers. Time-dependent density–density correlations in equilibrium dynamics show a two step relaxation that can be well fitted by stretched exponentials. While these results are important in showing that the FLG presents a qualitatively similar behavior as many real glass formers, it is important to note that glasses are essentially out of equilibrium systems with relaxation times spanning many orders of magnitude. Consequently, one should look at the out of equilibrium dynamics of the model in order to gain insight of the experimental behavior of glasses. A characteristic feature of glassy systems is their history dependence. The response to a perturbation applied at a particular time $t_w$ will persist for very long times, a phenomenon called *long-term memory*. This long-term memory prevents the system from reaching equilibrium and two times quantities like correlations and responses lose time translational invariance (TTI). In other words, two times quantities depend explicitly on the observation time and on the time when the perturbation was applied, this kind of behavior being known as *physical aging*. Aging dynamics is present in the FLG both in density–density correlations as well as in correlations of

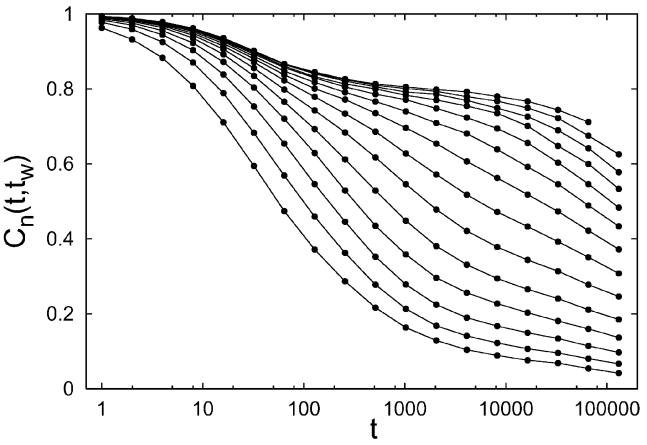


Fig. 1. Density autocorrelations after a quench to $\mu = 10$ at $T = 1$ and $J = 10$ for $L = 20$. The waiting times range from $2^5$ (bottom) to $2^{17}$ (top) and the averages are over 50 samples.

the internal degrees of freedom [10,16] after performing sudden quenches in the value of the chemical potential from a very small value characteristic of the liquid phase to a high value corresponding to the glassy phase. Performing a quench in $\mu$ is similar to the application of a sudden compression, we raise the density of the system keeping the ratio $\mu/J \ll 1$ in order to prevent close packing. From Fig. 1 we note that for waiting times of the order of $2^{15}$ or greater and small observation times, the system enters a quasi-equilibrium regime (TTI approximately holds), falling out of equilibrium for longer time scales of the order of $t_w$. This 3D lattice has linear size $L = 20$ so one immediately notes that it will be very difficult, if at all possible, to reach equilibrium in the glassy phase. This is more clearly seen when one observes the evolution of the density as the chemical potential is slowly increased.

In Fig. 2 we see that for $\mu \geqslant 1$ the density depends on the cooling rate. Cooling at slower rates allow the system to reach greater densities, slowly approaching a limiting density near $\rho \approx 0.67$ as the cooling rate gets slower. This cooling rate dependence is another characteristic feature of structural glasses. The true equilibrium density would be attained at an infinitely slow cooling. On extrapolating our asymptotic values to zero cooling rate we obtain a $\rho_{\mathrm{eq}} \approx 0.68$. This behavior should mean that true equilibrium is practically avoided in this system. This resembles what is found in the spherical $p$-spin spin glass. In that system, after a quench from a high temperature to a sub-critical one, the energy relaxes not to the equilibrium value, but to a threshold value greater than that of equilibrium. In the thermodynamic limit $\mathcal{O}(N)$ barriers prevent the system from escaping these "threshold" states, true equilibrium is never achieved and the system ages forever [11]. In the present model an asymptotic value of the density smaller than the equilibrium one would indicate that a similar mechanism as in the $p$-spin model is at work. We must note, however, that contrary to what happens in the $p$-spin, in our model activated dynamics may be present and, in a finite system equilibrium eventually

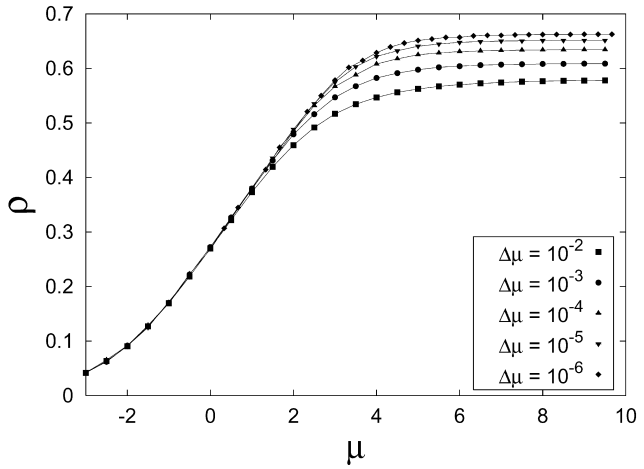


Fig. 2. Cooling rate dependence of the density. The value of the chemical potential $\mu$ is increased by $\Delta\mu$ at each MCS. The linear size is $L = 6$.

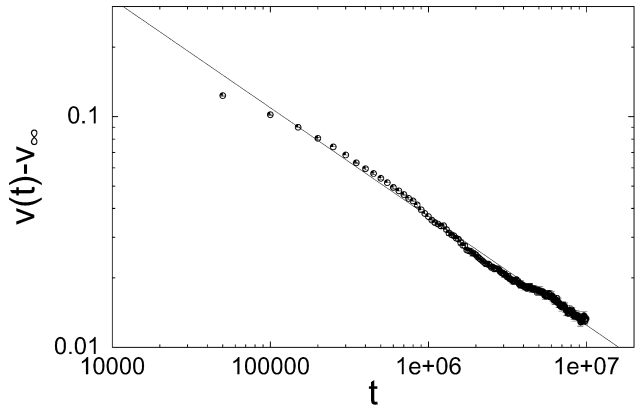


Fig. 3. Decay of the specific volume after a quench to $\mu = 10$ for a lattice with $L = 6$. The solid line is a power law fit over the last two decades. $v(t) = v_\infty + at^{-\alpha}$, with $\alpha \approx 0.47$ and $v_\infty = 1/\rho_\infty \approx 1.48$ ($\rho_\infty \approx 0.673$).

will be reached. In order to test this possibility we followed the time evolution of the density after a quench in a small sample with $L = 6$. Up to the times of the order of $10^7$ MCS the density is relaxing slowly to an asymptotic value $\rho_\infty \approx 0.673$ in close agreement with the finite cooling rate experiments as shown in Fig. 3.

Finally, we show results from aging simulations performed at constant density. In this system this corresponds to fixing the chemical potential and performing a quench in temperature. In Fig. 4 we see the decay of density autocorrelations at a constant density $\rho = 0.67$. This density was chosen as being a little smaller than the presumed threshold value. As expected, in this case the system can explore more efficiently the entire phase space and the dynamics soon becomes ergodic with TTI. Conversely in

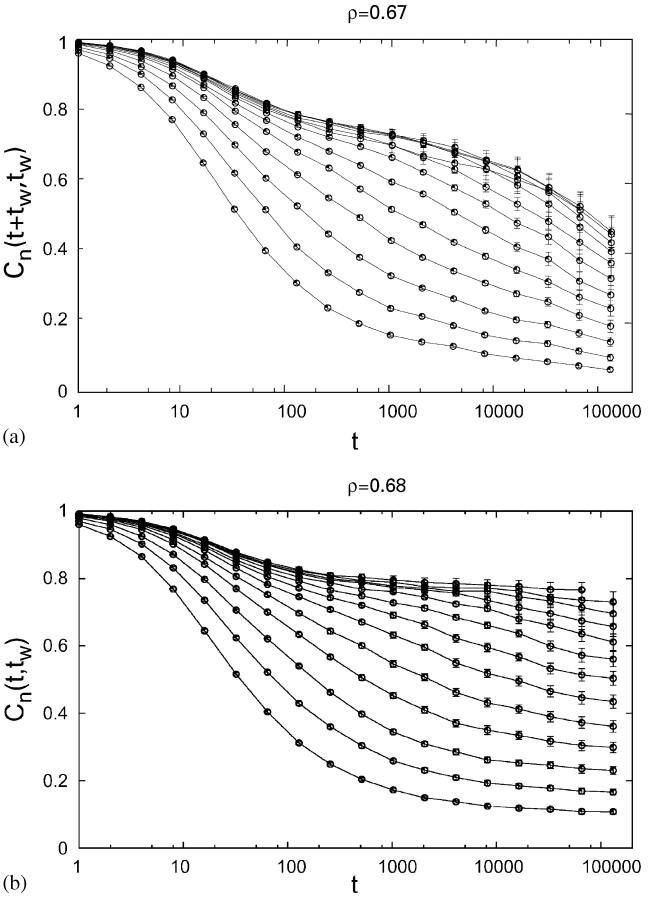


Fig. 4. Decay of the density autocorrelations after a quench at a constant density. Note that for $\rho = 0.67$ and moderate waiting times the dynamics becomes stationary and aging stops.

an equivalent simulation with fixed density $\rho = 0.68$, i.e., slightly above the threshold, the system gets frozen and the correlations do not decay to zero in finite timescales for large waiting times (see Fig. 4). This again is similar to what happens in the $p$-spin model when one fixes the energy of the system in values above and below the threshold, respectively. In a system which does not present this kind of behavior, e.g. the Sherrington–Kirkpatrick spin glass, this abrupt change around a particular energy is not expected to occur.

A crucial test for the possible $p$-spin like behavior of the frustrated lattice gas is the characterization of the so-called "fluctuation–dissipation ratio" [12]. The exactly solvable spherical $p$-spin is characterized by a constant value of this quantity. A constant value is characteristic of systems with one step of replica symmetry breaking (1RSB) and it is believed that real glasses should behave this way. Work in progress indicates that the FLG presents a constant FDT ratio [13,16]. It would be interesting to obtain

a mean field limit of this model where analytic calculations can be accessible. Some work in this direction has already been done [14,15].

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## References

[1] Science 267 (1995).
[2] W. Kob, J.L. Barrat, Phys. Rev. Lett. 78 (1997) 4581.
[3] K.H. Fischer, J.A. Hertz, Spin Glasses, Cambridge University Press, Cambridge, 1993.
[4] J.P. Bouchaud, L.F. Cugliandolo, J. Kurchan, M. Mézard, in: P. Young (Ed.), Spin Glasses and Random Fields, World Scientific, Singapore, 1998.
[5] J.P. Bouchaud, L.F. Cugliandolo, J. Kurchan, M. Mézard, Physica A 226 (1996) 243.
[6] A. Coniglio, Nuovo Cimento D 16 (1994) 1027.
[7] A. Coniglio, Philos. Magn. B 77 (1998) 213.
[8] M. Nicodemi, A. Coniglio, J. Phys. A 30 (1997) L187.
[9] M. Nicodemi, A. Coniglio, Phys. Rev. E 57 (1998) R39.
[10] D.A. Stariolo, J.J. Arenzon, Phys. Rev. E 59 (1999) R4762.
[11] L. Cugliandolo, J. Kurchan, Phys. Rev. Lett. 71 (1993) 173.
[12] L. Cugliandolo, J. Kurchan, L. Peliti, Phys. Rev. E 55 (1997) 3898.
[13] F. Ricci-Tersenghi, J.J. Arenzon, D.A. Stariolo, Phys. Rev. Lett. 84 (2000) 4473.
[14] J.J. Arenzon, M. Nicodemi, M. Sellitto, J. Phys. 6 (1996) 1143.
[15] M. Sellitto, M. Nicodemi, J.J. Arenzon, J. Phys. 7 (1997) 45.
[16] J.J. Arenzon, F. Ricci-Tersenghi, D.A. Stariolo, preprint.