On the scenario for the glass transition

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In this letter we study a lattice glass system that undergoes a glass transition. When we approach the glass transition we find both a divergence of a point to set correlation length and a vanishing of the thermodynamic potential. These findings are similar to the predictions coming from mean-field (replica) theory, but they differ from these predictions in some details: they underline the need of a better theoretical understanding of the glass transition.

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Second order phase transitions are usually characterized by the existence of an equilibrium correlation length that is divergent at the phase transition point. It is usually stated that such a correlation length is absent for the glass transition. However it was noticed long time that in the framework of the Adams Gibbs theory [1, 2, 3] the slow dynamics is dominated by large regions that move in a cooperative way. This observation has been formalized by introducing the appropriate correlations functions that can be used to define the dynamical correlation length [4, 5, 6, 8, 9]. A precise theoretical analysis has been done both in the framework the replica approach [6, 7, 10, 11, 12] and in the framework of the mode-coupling theory [13].

It was later realized that we can define a static correlation length that is divergent at the transition temperature [11, 12, 13, 14, 15]. It is related to the point to set correlations: its definition is the following. We start from a large system at equilibrium: we froze it and we allow only a region of size $R$ to move. We ask if the equilibrium configuration satisfying this constraint is very far from the original configuration. It is natural to suppose that if $R >> \xi$ the behaviour should be present for $R << \xi$. We can define an equilibrium correlation length $\xi_s$ as the minimal size of a non blocked region: the previous arguments suggest that we should have $\xi_s \propto \xi_d$. It has been shown [11] that in the mean field approach $\xi_s$ diverges near the transition point. While real experiments to measure $\xi_s$ are not yet feasible, numerical experiments have been done showing evidence of a large increase of the $\xi_s$ near the thermodynamic transition point [15].

In this letter I will study a different correlation length $\xi_w$. The definition is similar to $\xi_s$, but it is technically different [16]: we froze the system on a wall (a two dimensional slice) and we measure how the final configuration is different from the initial one (the geometry is similar to the one used in [17] for the dynamics). More precisely we introduce an overlap $q$ that indicates the similarity of two configurations: $q = 1$ for identical configuration while $q$ takes a small value for unrelated configuration. In this way, if we froze the region where $0 < x < 1$, $x$ being one of the coordinates, we can define the average value of $q$ at given $x$, i.e. $\bar{q}(x)$. The wall correlation length is defined by

$$q(x) = a \exp(-x/\xi_w) + q_{\text{bulk}}$$

(1)

at large $x$. The correlation length $\xi_w$ is logically different from $\xi_s$ and its behaviour in mean field theory is not clear.

In this letter we present evidence that the correlation length $\xi_w$ is divergent when we approach the phase transition in a lattice glass model (a similar conclusion has been reached for an off lattice fluid [16]). We will relate the divergence of $\xi_w$ to the development of flat direction for an appropriate thermodynamic potential [18].

The model we consider is a simple lattice gas model (the CTCC model [19]), that does not easily crystallize in simulations (the cell crystal contains $7^3 = 343$ particles and it is quite difficult to form). Each site of a three dimensional cubic lattice may be empty or occupied. If the site is occupied we have to specify the orientation of the particle. The particles may point in each of the six directions that correspond to elementary moves on the lattice. The system satisfies the constraints: 1) each lattice point may occupied by only one kind of particles,
2) if the site \( \vec{i} \) is occupied by a particle that points in the direction \( \vec{d} \), the site \( \vec{i} + \vec{d} \) is empty.

We introduce a chemical potential \( \mu \). In the limit \( \mu \to \infty \) we reach the maximum density state, i.e. a crystal with periodicity 7 and density \( 6/7 = 0.8571 \). In simulations on large lattices, starting from the disorder phase, there is no sign of crystallization up to the longest runs. One observes in the dynamics a very nice slowing down, with all the standard stigmata of a glass transition, i.e. mode-coupling behaviour of the correlation function (with both the \( \alpha \) and the \( \beta \) region well exposed), a strong increase of the dynamical susceptibilities and a simultaneous decrease of the diffusion constant \( D \). This data on the diffusion constant do not have a particular meaningful behaviour as function of the chemical potential \( \mu \).

The shape of the function \( \xi \) near the wall is an interesting problem that we do not address here. We focalize our interest on the behaviour at large \( x \). We find that for \( x \geq 2 \) the function \( q(x) \) can be remarkably well fitted by an exponential, i.e.

\[
q(x) - q_{\text{bulk}} = a \exp(-x/\xi_w) + c
\]

where \( c \) is a small constant, i.e. \( O(10^{-3}) \) (the previous hand-waving argument suggest that \( \xi_w \) should diverges at the thermodynamic phase transition where \( \xi_w \) diverges).

An example of the fit is shown in fig. 1, where the data are taken at \( \mu = 8.5 \) (\( \rho = 0.810 \)) on a cubic lattice of side \( L = 22 \). The value of the correlation length is \( 1.32 \pm 0.03 \).

We have measured this correlation (or penetration) length \( \xi_w \) in the region of \( \mu \) ranging from 1 to 9.25 on lattices of various side (up to \( L = 28 \)). The correlation \( \xi_w \) is very well fitted by a power low behaviour

\[
\xi_w(\rho) = A(\rho_c - \rho)^\nu,
\]

with \( \rho_c = 0.826 \pm 0.002 \) and \( \nu = 0.48 \pm 0.02 \) (see fig. 2).

In the study of phase transitions one usually introduces an order parameter and an associated thermodynamic potential. If the order parameter is a continuos function of the temperature, at the phase transition point the potential is zero only in one point, while at lower temperatures it is different from zero in a region whose side goes to zero at the critical point. For a transition with a discontinuous order parameter, at the phase transition point the potential is zero when the order parameter stays in a given interval and a similar behaviour is present also below the phase transition point. In the infinite volume limit the potential must be convex function: when the potential is not convex in a mean field approximation, Maxwell construction enforces the convexity.

The glass transition may be characterized by the existence of regions of configuration space where (below the transition) the system remains trapped for an infinitely long time. The overlap \( q \) is the putative order parameter.
With probability one when the volume $V$ goes to infinity, the potential $W(q)$ does not depend on the reference configuration $\sigma$. In other words $P_\sigma(q) \approx \exp(-VW(q))$. By construction $W(q_{\text{bulk}}) = 0$ and the vanishing of the potential $W(q)$ for more than one $q$-value is the distinctive characteristic of replica symmetry breaking (it should occur below the thermodynamic glass transition).

There are many possible techniques that can be used to compute the potential $W(q)$. One of the best is the introduction of a tethering potential, as described in [24].

Here we use a simpler method [23]: we constrain the $\tau$ configuration to stay in the region $q_{\sigma,\tau} > q^*$. With this constrain the resulting probability distribution of $q_{\sigma,\tau}$ is proportional to $\theta(q-q^*) \exp(-VW(q-q^*))$. In the region where $q^* > q_{\text{bulk}}$, we have that

$$V(q_{\sigma,\tau} - q^*) = \left( \frac{dW}{dq} \right)^{-1} = 1/W'(q^*) \quad (7)$$

Using a wild metaphor we could say that $W'(q)$ corresponds to the force that pushes the system away from the region where $q$ is high. It is interesting to note that in the Maxwell construction $W'(q)$ is constant in the region where the naive mean field prediction violates convexity.

In the replica approach to glasses the potential $W(q)$ plays a central role [4]: in the mean field approach at high temperature the potential is convex. By decreasing the temperature firstly the convexity is lost; at a lower temperature (i.e. at the dynamic or mode-coupling transition) a secondary local minimum $(q_m)$ appears. The height of the minimum (i.e $W(q_m)$) is the configurational complexity $\Sigma$. By decreasing the temperature the value of $W(q)$ at the secondary minimum decrease up to the point (the Kauzmann transition) where $W(q_m) \equiv \Sigma = 0$. Below this temperature we are in the glass phase: two minima (with $W(q) = 0$) are present and the replica symmetry is broken. This scenario is valid in infinite range model where very detailed computation can be done.

It is clear that the previous picture must be strongly modified in finite dimensions. We have already remarked the any thermodynamic potential in the infinite volume limit must be convex. A consistent scenario could be provided by the Maxwell construction, unfortunately there are not many numerical result on the behaviour of the potential in finite dimensional models [6].

In this letter we compute the the potential $W(q)$ in the CTCC lattice gas model and we find that it has some surprising properties. The derivative of the potential $W'(q)$ at various densities (from 0.749 to 0.810) is shown in figs. [4] and [5]. A few remarks are in order:

- We cannot identify regions where $W'(q)$ decreases by increasing $q$: convexity is always strictly satisfied.
- There are no flat regions ($W'(q) = \text{const}$) that could be the remnant of the Maxwell construction. Therefore no dynamical (mode coupling) transition can be identified.
- The potentials at different densities have similar shape.
- The potential strongly decrease in nearly the whole $q$ interval when the density increases.

The last two statements can be done more sharply if we rescale the potential with the square of the correlation length

$$\Omega'(q) \equiv \xi_w(\rho)^2 W'(q) \quad (8)$$

FIG. 3: The same data as fig [2]: here we plot $\xi_w(\rho)^{-2}$ versus $\rho$ in a linear scale.

FIG. 4: The derivative of the potential $W'(q)$ at various densities (0.749, 0.771, 0.789, 0.803, 0.810) on large systems of side $L = 40$. 
The data for \( \Omega'_\rho(q) \) are shown in fig. 5 and they are weakly dependent on the density. If \( \xi_\omega(\rho) \) goes to infinity at a critical value of \( \rho \) the potential \( W(q) \) goes to zero in the whole interval from \( q_m \) up to a value of \( q \) of near to 0.9.

The results are surprising (at least to me) for the following reasons:

- The potential \( W(q) \) cannot be used to identify the (dynamic) mode coupling transition: the configurational complexity cannot be defined. However it is possible that in this model the dynamic transition is very near to the static one, so that the two transitions cannot be easily disentangled: is this case one may observing overlapping features. One should also remember that \( W(1) \) is the entropy. If at the Kauzmann transition the entropy takes a very small value, the potential \( W'(q) \) should be nearly vanishing in large interval of \( q \).

- The extrapolation of these results implies that a static Kauzmann transition is present and the behaviour is rather simple. The exponent \( \nu \) is very near to the simple value 1/2 and the thermodynamic \( W'_\rho(q) \) potential scales naively without any need of introducing extra power corrections.

Similar investigations are presently done also for off-lattice fluids and it would be very interesting to compare the results. A very important question is the theoretical derivation of these results.

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\[ \text{FIG. 5: The same data of fig. 4 for derivative of the potential } W'_\rho(q) \text{ multiplied by } \xi_\omega(\rho)^2, \text{ i.e. } \Omega'_\rho(q). \]

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