Different Scenarios for Critical Glassy Dynamics

S. Ciuchi\(^1\) and A. Crisanti\(^2\)

\(^1\) Dipartimento di Fisica, Università de L’Aquila and
Istituto Nazionale Fisica della Materia, Unità dell’Aquila
via Vetoio, 67100 Coppito-L’Aquila, Italy.

\(^2\) Dipartimento di Fisica, Università di Roma “La Sapienza” and
Istituto Nazionale Fisica della Materia, Unità di Roma
P.le A. Moro 2, 00185 Roma, Italy.

(received ; accepted )

PACS. 64.70.Pf – Glass transitions.
PACS. 75.10.Nr – Spin-glass and other random models.
PACS. 61.20.Gy – Theory and models of liquid structure.

Abstract. – We study the role of different terms in the \(N\)-body potential of glass forming systems on the critical dynamics near the glass transition. Using a simplified spin model with quenched disorder, where the different terms of the real \(N\)-body potential are mapped into multi-spin interactions, we identified three possible scenarios. For each scenario we introduce a “minimal” model representative of the critical glassy dynamics near, both above and below, the critical transition line. For each “minimal” model we discuss the low temperature equilibrium dynamics.

In the last years many efforts have been devoted to study the relaxation dynamics of undercooled liquids near the (structural) glass transition. When the temperature of the liquid is lowered down to the critical glass temperature relaxation times becomes exceedingly long and diffusional degrees of freedom freeze over very long time scales. As a consequence the difference between a structural glass and a disordered system with quenched disorder, which may seem essential, becomes less and less sharp as the transition is approached since the particles in the liquid become trapped in random position (cage effect) and the dynamics of a single degree of freedom resembles the relaxational dynamics in a random quenched potential. The idea that a undercooled liquid is a sort of random solid, which dates back to Maxwell\(^3\), has been recently largely used in the study of the glass transition in undercooled liquids. In this scenario is, for example, the study of the Instantaneous Normal Mode (INM)\(^4\), where the N-body potential is analyzed in terms of normal modes of oscillations about a given instantaneous configuration. Using this technique many properties of the N-body potential in models of undercooled liquids have been recently traced out\(^5\).

\(^{(*)}\) e-mail: sergio.ciuchi@aquila.infn.it
\(^{(**)}\) e-mail: andrea.crisanti@roma1.infn.it

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In this letter, based on the connection between structural glasses and quenched disorder models, we shall analyze from a general point of view the role of different terms in the $N$-body potential, such as local stress and other non-harmonic terms, on the critical dynamics. We are interested only in the general properties; therefore we shall use a simple spin-glass model where the different terms of the original $N$-body potential are mapped into multi-spin interactions.

In this spirit, local stresses are represented by a linear term, the harmonic part becomes a two-spin interaction term, and higher order nonlinear terms become $p$-spin interactions with $p > 2$. The use of spin models to study the (structural) glass transition, which dates back to the end of 80’s [7], has the great advantage that one can construct solvable spin models displaying the typical critical behavior of structural glasses [8, 9, 10]. The model we consider is a spherical spin-glass model with (random) potential

$$V[\sigma] = \sum_{p \geq 1} \left( \sum_{1 \leq i_1 < \cdots < i_p \leq N} V_{i_1 i_2 \cdots i_p}^{(p)} \sigma_{i_1} \sigma_{i_2} \cdots \sigma_{i_p} \right) + \sum_{p \geq 1} \sum_{1 \leq i_1 < \cdots < i_p \leq N} V_{i_1 i_2 \cdots i_p}^{(p)} \sigma_{i_1} \sigma_{i_2} \cdots \sigma_{i_p}$$  \hspace{1cm} (1)

where $V_{i_1 i_2 \cdots i_p}^{(p)}$ are uncorrelated zero mean Gaussian variables of variance

$$\left( V_{i_1 i_2 \cdots i_p}^{(p)} \right)^2 = \frac{J_p^2 p!}{2N^{p-1}}$$  \hspace{1cm} (2)

and $\sigma_i$ are $N$ continuous variables obeying the spherical constraint $\sum_i \sigma_i^2 = N$. The parameters $J_p$ define the relative strength of the various terms in (1) and can be tuned to reproduce some of the properties of the $N$-body potential of undercooled liquids obtained for instance by INM analysis. This model has been discussed to some extent in literature, see e.g. Refs. [8, 9, 10], as prototype mean-field model for the structural glass transition, and recently also to fit experimental data [11]. It is known that the high temperature phase is described by the (schematic) Mode Coupling Theory (MCT) for structural glasses. However, to our knowledge, a systematic analysis of the relation between the leading terms in the potential (1) and the critical dynamical behavior, similar to what done in MCT [15], was never done. Our analysis identifies three possible scenarios for critical dynamics, similar to what found in MCT, and allows for the introduction of a “minimal” spin-glass model for each scenario which describes the critical dynamics near, both above and below, the transition. We stress that while the high temperature phase is similar to what found in MCT, the low temperature phase is different. We finally note that our analysis also reveals all the possible scenarios for glassy transition that can be obtained with this model.

The relaxation dynamics is defined as usual by the Langevin equation

$$\partial_t \sigma_i = -R \sigma_i - \frac{\partial V[\sigma]}{\partial \sigma_i} + \xi_i(t)$$  \hspace{1cm} (3)

where $\xi_i(t)$ is a Gaussian random field (thermal noise) with variance $\langle \xi_i(t) \xi_i(t') \rangle = 2 \delta(t - t')$, $T = 1/\beta$ the temperature and $R$ a Lagrange multiplier to ensure the spherical constraint which must be fixed self-consistently. If only the linear term $p = 1$ and one term with $p > 2$ are present in the expansion (1), the model is equivalent to the spherical $p$-spin model introduced in Ref. [12] whose dynamics has been studied in Ref. [8, 16]. The case where only the quadratic term $p = 2$ is present has been analyzed in Refs. [17, 18]. It is worth noting that there is a nontrivial difference between the dynamics for $p = 2$ and $p > 2$. Indeed while in the former case relaxation is an orientation process of the state vector $\{\sigma_i\}$ toward a (doubly degenerate) state $\langle \sigma_i \rangle_0 $, for $p > 2$, similar to what happens in structural glasses, relaxation occurs in a free energy landscape characterized by many (highly degenerate) local minima $\langle \sigma_i \rangle_0 , \langle \sigma_i \rangle_1$. In this
spirit small non-harmonic terms change qualitatively the dynamical properties, therefore in this letter we always assume at least cubic nonlinearities.

The analysis of (3) simplifies considerably in the thermodynamic limit $N \to \infty$, where the dynamics can be described by a set of self-consistent equations involving a single spin only and the averaged correlation and response functions $C(t, t')$ and $G(t, t')$ \[20, 7, 9, 21\]. In the high temperature phase at equilibrium $C$ and $G$ are related by the fluctuation dissipation theorem (FDT) $G(t, t') = G(t - t') = -\theta(t - t')\partial_t C(t - t')$ and the the mean-field dynamical equation simplifies further, for details see e.g. Refs. \[20, 7, 9, 21\]. The resulting mean-field dynamical equation can be written as,

$$[\partial_t + \tau] C(t) + \int_0^t ds \Lambda(t - s) \partial_s C(s) = 1 - \tau \quad (4)$$

where $\Lambda(t) \equiv \Lambda[C(t)] = \sum_{p \geq 2} \mu_p C^{p-1}(t)$, $\tau = R - \sum_{p \geq 2} \mu_p$, $\mu_p = J_p^2 p^2 / 2T^2$, and $t$ is now a time difference. For large $t$ we can define the Edward-Anderson order parameter as $\lim_{t \to \infty} C(t) = q_0$ which, taking the $t \to \infty$ limit of eq. (4), obeys the equation:

$$\mu_1 + \Lambda[q_0] = \frac{q_0}{(1 - q_0)^2} \quad (5)$$

The parameter $\tau$ has been eliminated using the the spherical constraint which now reads $C(0) = 1$. This is the “replica symmetric” solution for this model. Stability analysis reveals that this solution is stable iff

$$\frac{d\Lambda[q_0]}{dq_0} \leq \frac{1}{(1 - q_0)^2} \quad (6)$$

the equality being satisfied along the transition line. Since the linear term in \[1\] acts as an external field, it can be shown that if $\mu_1 = 0$ the only stable solution is $q_0 = 0$ while for $\mu_1 > 0$ we have $0 < q_0 < 1$ \[3\]. The order parameter $q_0$ is the time-persistent part of the correlation induced by the variance of the local stress, therefore $q_0 \neq 0$ is not associated to a glassy phase. We note that in structural glasses has been found \[22\] that local stresses develop a zero mean Gaussian distribution approaching the glass transition, therefore even if their role is irrelevant well inside the liquid phase, they can be relevant for the dynamical transition. To study the relaxation near the transition we introduce the (rescaled) connected correlation function $\phi(t)$ by writing $C(t) = q_0 + (1 - q_0)\phi(t)$ where, from eq. \[4\] and \[3\], $\phi(t)$ obeys the equation

$$\partial_t \phi(t) + \frac{1}{1 - q_0} \phi(t) + \int_0^t ds \Delta\Lambda(t - s) \partial_s \phi(s) = 0 \quad (7)$$

with $\phi(0) = 1$ and

$$\Delta\Lambda(t) = \Lambda[C(t)] - \Lambda[q_0] = \sum_{k=1}^\infty \lambda_k \phi^k(t) \quad (8)$$

$$\lambda_k = \frac{(1 - q_0)^k}{k!} \frac{d^k}{dq_0^k} \Lambda[q_0]. \quad (9)$$

This equation has the same structure of the schematic MCT equation for glasses considered by Götze \[23\]. The factor $(1 - q_0)^{-1}$, absent in the Götze equation, just changes the form of the long time solution near the type B transition (see below). The Götze equation is recovered for $q_0 = 0$. 


In deriving eq. (7) we made use of FDT so that this equation is appropriate only above the dynamical transition. In the low temperature phase (spin-glass or glass phase) the FDT must be modified \[9, 16\] and, moreover, non-equilibrium \[16\] and equilibrium \[9\] dynamics are separated by infinite time scales and described using different approaches.

The transition from the high to the low temperature phase is of type A or B depending on the instability of eq. (7). The type A transition occurs along the instability line of solution (5) [equal sign in eq. (6)] and is the analogues of the De Almeida and Thouless line in spin glasses. Type B transition appears with a sudden appearance of another long time persistent solution: \( \lim_{t \to \infty} \phi(t) = f \neq 0 \) where, from eq. (7), \( f \) is solution of the bifurcation equation: \( \Delta \Lambda[f] = f[(1-q_0)(1-f)]^{-1} \). For \( q_0 = 0 \) this reduces to that found by Götte \[23\]. Defining \( f = (q_1 - q_0)(1-q_0)^{-1} \) we recover the usual equation for \( p \)-spin-like models at the discontinuous transition \[3, 21\]. The relaxation dynamics near the two types of transitions is quite different, as shown schematically in Fig. 1 where relaxation parameters are defined.

Which kind of transition – type A or B – takes place depends on the parameters \( \mu_p \). Near the transition only the first two non-zero terms in the sum (1) are relevant, all others giving sub-leading corrections which can be neglected at the transition. The six non-trivial cases are reported in table \( \text{I} \). All other cases can be qualitatively mapped to one of these. With \( \mu_{p>3} \) we mean a generic non-harmonic term of order \( p > 3 \). The six cases can be grouped into three different classes depending on the two relevant \( \lambda_k \). Following a notation introduced by Götte, we call them \( 1-2, 1-3 \) and \( 2-3 \), respectively. For each class we can define a “minimal” spin-glass model obtained by retaining only two terms in the sum (1). If we denote these modes with \( x+y \)-SG model, where \( p = x, y \) are the two retained terms, the simplest choice for spin-glasses “minimal” model is: \( 2+3 \)-SG model for class \( 1-2 \), \( 2+4 \)-SG model for class \( 1-3 \)
and $3 + 4$-SG model for class 2 - 3 [table I]. With this choice the relation between $\mu$'s and $\lambda$'s is very simple: $\lambda_k = \mu_{k+1}$. One could use other choices, e.g. the $1 + 3$-SG model for the class $1 - 2$. This would lead to a different relation between $\mu$'s and $\lambda$'s, but will not change the results if expressed in terms of $\lambda$'s.

The “minimal” models can be analyzed in full details also far from the transition and hence can be used to gather more informations on the low temperature phase in the different classes. For this reason in what follow we shall restrict to the “minimal” models and consider the equilibrium dynamics in the low temperature phase. In is clear that the results we shall obtain are also valid for the full model as far as the extra terms in potential $V$ can be neglected, i.e., only near the transition. The equilibrium dynamics in the low temperature phase can be studied using the technique of Ref.[20, 9] which assume equilibration on very long times and a modified form of FDT for the very slow processes. This method is known to reproduce the low temperature phase statics. The calculation is lengthy and will not be reported. Here we quote the main results. The non-equilibrium aging phenomena can be studied using the technique of Ref. [16], but these are beyond the purpose of this paper.

In Fig. 2 (a) we report the phase diagram in the $\lambda_1 - \lambda_2$ plane of the “minimal” $2 + 3$-SG model. This is equal to the phase diagram of the spherical $p$-spin model in a field [8, 9] when expressed in terms of $\lambda_1, \lambda_2$. For small $\lambda_2$ a transition of type A separates a paramagnetic from a glassy phase described by “1-step” replica symmetry broken solution. By increasing $\lambda_2$ along the critical line $\lambda_1 = 1$ we eventually reach a tricritical point where the type B solution appears and the transition changes from A to B. Since $f$ is zero at this point there is no jump in the bifurcation parameter. As far as the transition lines are concerned, this phase diagram is similar to what obtained in MCT for structural glasses [23], however the properties of the low temperature phase are different [8, 9].

The phase diagram of the “minimal” $2 + 4$-SG model, shown in Fig. 2 (b), is more reach. The high temperature phase is still separated from the low temperature phase by a type A transition for small $\lambda_3$ and by a type B transition for higher $\lambda_3$. However the low temperature phase consists now of two different glassy phases: one described by “1-step” and one by “$\infty$-steps” replica symmetry broken solution. The transition from 1-step to $\infty$-steps RSB appears as an instability of the 1-step RSB phase – type A – and in this respect is similar to what found for the Ising $p$-spin model [24]. The point where the type A and type B transitions meet is not a critical point since the two lines just cross, and $f$ jumps discontinuously. The possibility of two different glassy phases in model (1) was discussed in Ref.[12], however the properties of the low temperature phase are different [8, 9].

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| $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_{p>3}$ | $\lambda_1$ | $\lambda_2$ | $\lambda_3$ |
|--------|--------|--------|-------------|-------------|-------------|-------------|
| 0      | 1      | 1      | -           | 1           | 1           | -           |
| 1      | 1      | 1      | -           | 1           | 1           | -           |
| 1      | 1      | 0      | 1           | 1           | 1           | -           |
| 1      | 0      | 1      | -           | 1           | 1           | -           |
| 0      | 1      | 0      | 1           | 1           | 0           | 1           |
| 0      | 0      | 1      | 1           | 0           | 1           | 1           |

Table I. – 0 = missing, 1 = present , - = irrelevant
Fig. 2. – The phase diagram of the “minimal” 2 + 3-SG model (a), and of the “minimal” 2 + 4-SG model (b). The exponents of $C(t)$ [see Fig. 1] and the value of $f$ are shown at the edges of the transition lines.

is not appropriate for our model.

The “minimal” 3 + 4-SG model is the simpler one since the absence of quadratic term in the potential makes the continuous transition impossible [12]. A discontinuous transition of type B separates the high temperature phase form a low temperature phase of “1-step” RSB type, see Fig. 3.

In conclusion in this Letter we have shown that simple multi-spin interactions spin-glass spherical models, which obeys MCT equations above the dynamical transitions, lead to three different scenarios for critical dynamics according to the leading terms in the potentials. The type of dynamical transitions can be continuous as well as discontinuous. From a general point of view a continuous transition may occur only if harmonic and/or linear terms are important. Within the assumption that different terms of the real $N$-body potential of glass-forming systems can be mapped into the multi-spin interaction terms in (1), using the informations from INM studies the type of scenario for the critical dynamics can be predicted.

Schematic models of MCT for structural fragile glasses and undercooled liquids belong to the 1 − 2 class of universality. This is in agreement with our conclusions since in these systems local stresses and cubic nonlinearities are known to be important [3]. Based on the same assumptions the continuous transition observed in the rotational dynamics of linear molecules [25, 24] could be related to the relevance of linear and/or harmonic terms in the rotational degrees of freedom potential. To test our conjectures it would be also of interest to find physical systems belonging to 1 − 3 or 2 − 3 dynamical universality class.

To get more insight on the low temperature phase for each scenario we have introduced a
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Fig. 3. – The phase diagram of the “minimal” 3+4-SG model. The exponents of $C(t)$ [see Fig. 1] and the value of $f$ are shown at the edges of the transition lines.

“minimal” SG model and discussed the equilibrium low temperature dynamics. In particular for the 1−3 class has been calculated the critical transition line between the two glassy phases. The results found for the “minimal” models do apply to the full model near the transition lines, both above and below the transition. Recent results [27] have shown that finite-size mean-field $p$-spin-like models, where activated processes are allowed, exhibit strong similarities with structural fragile glasses. Therefore the “minimal” models can be highly valuable to study the glass transition in the different scenarios also beyond MCT. Work in this direction is in progress.

We finally stress that there are examples of glass forming systems where the MCT scenario is different from those proposed in the present Letter. For example a mixture of sticky hard-sphere exhibits a two different glass phase separated by a type B transition [28]. In this case the short wave-length dependence of vertices in the MCT plays a crucial role and therefore a simple model where inhomogeneous spatial fluctuations are neglected, as the one considered in this Letter, cannot be used.

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We wish to thank A. Cavagna, C. Donati, F. Sciortino and P. Tartaglia for valuable discussions and critical reading of the manuscript.

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