Numerical study of a short-range $p$-spin glass model in three dimensions

Matteo Campellone*, Barbara Coluzzi** and Giorgio Parisi**

March 24, 2022

March 24, 2022

(*) Departament de Física Fonamental
Universitat De Barcelona
Diagonal 647, Barcelona, Spain
(**) Università di Roma “La Sapienza”
Piazzale A. Moro 2, 00185 Rome (Italy)
e-mail: campellone@roma1.infn.it, coluzzi@roma1.infn.it, giorgio.parisi@roma1.infn.it

Abstract

In this work we study numerically a short range $p$-spin glass model in three dimensions. The behaviour of the model appears to be remarkably different from mean field predictions. In fact it shares some features typical of models with full replica-symmetry breaking (FRSB). Nevertheless, we believe that the transition that we study is intrinsically different from the FRSB and basically due to non-perturbative contributions. We study both the statics and the dynamics of the system which seem to confirm our conjectures.

PACS Numbers 05-7510N

1 Introduction

One of the presently unsolved theoretical issues concerning spin glasses is to obtain a satisfying description of these systems in finite dimension. By now, a quite complete picture has been achieved for spin glass models at mean field level [1]. Quite generally, one finds a critical
temperature $T_c$ which separates an ergodic phase from a low temperature spin glass phase in which ergodicity is broken. Below $T_c$ the spins are frozen in their local orientation, giving rise, because of the disordered nature of the interactions, to no total spontaneous magnetization.

This transition is well described by a spontaneous replica symmetry breaking scheme [1]. In the replica framework the order parameter of the spin glass transition is a function $q(x)$ defined on the real interval $[0, 1]$ that changes from a high temperature constant form $q(x) = q_0$ to a low temperature function that can assume different values. The physical meaning of the function $q(x)$ is the following: at low enough temperatures the free energy landscape has many local minima separated by free energy barriers that grow, asymptotically, as the size of the system. Below the critical temperature the system breaks the ergodicity and remains confined into one of these valleys. The values assumed by the order parameter function $q(x)$ are the possible values of the overlap $q_{\sigma\tau} = N^{-1} \sum_i^N \sigma_i \tau_i$ among two copies (replicas) of the system which are independently equilibrated in the same free energy landscape.

If the two replicas freeze into the same pure state then the overlap will be the maximum allowed ($q_{EA}$) and it will provide a measure of the width of the state. The size of the interval where $q(x) = q$ gives the probability that the two replicas are found with an overlap $q$. More precisely, one can define a quantity $P(q) = \frac{dx(q)}{dq}$ where $x(q)$ is the inverse function of $q(x)$. The function $P(q)$ is the probability distribution of the values of the overlap and it contains the same amount of information as the $q(x)$. At high temperatures one has a constant $q(x) = q_0$ which means that the $P(q)$ is a delta function on $q_0$.

Two main classes of spin glass models can be distinguished depending on the character of their phase transition.

- A first class of models undergoes, in mean field, to a full replica symmetry breaking (FRSB) transition in which the function $q(x)$ changes continuously with the temperature. The low temperature solution is a continuous function in which all values of the overlap between $q_0$ and $q_{EA}$ are attained. Correspondingly, the $P(q)$ will change to a non-zero continuous function between $q_0$ and $q_{EA}$ with an additional delta function on $q_{EA}$.

This transition is continuous in the sense that $q_{EA} - q_0$ is small for $T$ close to $T_c^-$. These models describe with success the physics of real spin glasses. This kind of transition is second order. At a critical temperature $T_c$ the spin glass susceptibility diverges and long range correlations establish.

- A second class of spin glasses has a discontinuous low temperature function $q(x)$ that can assume a finite number of values. Usually $q(x)$ assumes only two values $q_0$ and $q_1 (= q_{EA})$ and the transition involves one step of replica symmetry breaking (1RSB). In most cases the transition is discontinuous in the sense that $q_0 - q_{EA} \simeq O(1)$ as soon as $T < T_c$.

The low temperature $P(q)$ can be written in the following form

$$P(q) = m\delta(q_0) + (1 - m)\delta(q_1)$$

where $m$ is a parameter which is smaller than unity and it decreases with the temperature.
In this second class of models the distribution $P(q)$ is zero between $q_0$ and $q_1$ which are the only allowed values for the overlap. This is very different from the case of models of the first class where the low-temperature $P(q)$ shows a plateau from zero to $q_{EA}$ and there is no $\delta(q_0)$. In absence of magnetic field one always has $q_0 = 0$. We shall stick to this case in the following.

Another important feature of mean field spin glasses is that the dynamical equations for the two-time correlation functions show a singularity at a critical temperature $T_d \geq T_c$. It turns out that for models of the first class the dynamical and statical critical temperatures coincide, while in models of the second class one has $T_d > T_c$. The existence of a dynamical singularity at a higher temperature than the static critical temperature is an aspect of these models which is shared by structural glasses [2].

The mode-coupling (MC) theory describes quite well the dynamics of supercooled liquids [3] approaching their structural glass transition. The MC dynamical equations predict a singularity at a temperature $T_{mc}$ which is higher than the glass temperature $T_g$ predicted for real glasses in a static Adam-Gibbs scenario.

There has been recent effort to approach the structural glass transition by means of the techniques developed for disordered systems such as spin glasses [4, 5]. An effective disorder is in fact induced in structural glasses by the slow dynamics of the microscopic variables.

So, despite the absence of quenched disorder in the Hamiltonian and the possible presence of a crystalline groundstate (which however corresponds to a golf-shaped minimum in the free-energy landscape and can therefore been considered irrelevant to the physics of the system), it is believed that the behaviour of structural glasses is very similar to the one of 1RSB mean field spin glass models. Recent numerical results seem to support this hypothesis [3]-[6]. Of course, in finite dimensional glasses, the effect of the decay of metastable states by activated processes have to be taken into account, and are an element of difference with respect to mean field spin glasses. An interesting issue is to generalize long range models of spin glasses with 1RSB to models with short range interactions to see if the finite dimensional effects are similar to the case of real glasses or not.

In this work we present a numerical study of a 3d short-ranged version of the $p$-spin model [11, 12, 13, 14]. The model is provided of a parameter $M$ that ensures the mean field solution to be exact when $M$ is sufficiently large. A perturbative analysis around the mean field solution predicts a behaviour qualitatively similar to the MF [11]. Nevertheless, numerical simulations give evidence for a diverging correlation length when approaching the critical temperature from above [12].

We study the model in $d = 3$ for $p = 4$ and $M = 3$. We look at the behaviour of the function $P(q)$ which appears definitely non trivial at low temperatures. The form of the $P(q)$ that we find seems to be relevantly different from the shape that one has in the case of the mean field $p$-spin model. Our results indicate the occurring of a continuous transition. Furthermore, a numerical study of the dynamics of this model seems to provide evidence for a dynamical transition at the same critical temperature of the static one as in the cases of models with a continuous transition. Nevertheless we believe that this transition is very peculiar and is not due to an instability of the saddle point as in the case of models with FRSB. We address
the peculiar nature of this transition to the formations of large regions of highly correlated
spins which are localized by the quenched disorder and whose typical size grows as $T \to T_c$.
Before presenting the short range model and our numerical results, we will devote the following
section to describing the known results for the 1RSB class of mean field spin glasses and to
do so we will focus on a particularly simple model belonging to this class.

2 The long-range $p$-spin glass model

In this section we shall briefly resume the known results for a long range model that has been
extensively studied in the past and, because of its simplicity, is a recommendable paradigm
for mean field spin glasses undergoing a 1RSB transition.

The model in zero magnetic field is defined by the $p$-spin interaction Hamiltonian

$$H_p(\{\sigma\}) = - \sum_{(1 \leq i_1 < i_2 < \cdots < i_p \leq N)} J_{i_1,i_2,\ldots,i_p} \sigma_1 \cdots \sigma_p.$$ (1)

The spin variables can be either Ising spins ($\sigma_i = \pm 1$) or continuous soft spin variables
which have to be constrained by some normalizing condition such as

$$\sum_{i=1}^{N} \sigma_i^2 = N,$$ (2)

where the interactions $J_{i_1,i_2,\ldots,i_p}$ are random variables distributed with

$$P(J_{i_1,i_2,\ldots,i_p}) = \left[ \frac{N^{p-1}}{\pi J^{2p}} \right]^{-\frac{1}{2}} \exp \left[ - \frac{(J_{i_1,i_2,\ldots,i_p})^2 N^{p-1}}{J^{2p}} \right].$$ (3)

The scaling of the variance with $N^{p-1}$ ensures the free energy to be extensive. The mean
field solution of the model is exact when the limit $N \to \infty$ is taken since the interactions are
long ranged. The physics of the Ising and of the spherical $p$-spin glass model is essentially the
same if $p > 2$. Here we will review some well established results in the spherical case which
can be exactly solved. For $p = 2$ this model does not belong to the 1RSB class, and exhibits
a continuous transition.

The model presents a 1RSB discontinuous transition at a temperature $T_c$. One can dis-
tinguish two other relevant temperatures $T_d$ and $T_m$, where

$$T_c < T_d < T_m.$$ (4)

The physics of the model is characterized by the appearance of a large number of solutions
different from the paramagnetic one. We can schematically resume the behaviour of the model
with respect to temperature as follows

- For $T > T_m$ the model is in a paramagnetic phase which is the only minimum of the free
energy.
• For $T_d < T < T_m$ the free energy landscape changes. The physics of the model is still dominated by the paramagnetic state, but other local minima of the free energy appear. These minima have a lower energy than the paramagnetic state but their free energy is higher and therefore they are still irrelevant in the thermodynamic limit. There is an exponential number of these minima. One can define the complexity $\Sigma$ as the logarithm of the number of states that becomes extensive below $T_m$.

The free energy of the ensemble of these states is therefore

$$\mathcal{F}_s = E_s - TS - T\Sigma$$  \hspace{1cm} (4)

Above $T_d$ one has $F_s > F_p$ where $F_p$ is the free energy of the paramagnetic state. So in this regime the dominant solution is still the paramagnetic one.

• In the whole range of temperatures such that $T_c < T < T_d$ one finds that the free energy of the paramagnetic state equals the free energy of the ensemble of local minima i.e.

$$\mathcal{F}_s = F_p.$$  

It turns out that at the temperature $T_d$ the solutions to the dynamical mean field equations change. In this sense $T_d$ is the dynamical critical temperature. This corresponds to the fact that, if the system starts from a random initial configuration, the system will eventually fall into a metastable state where it will be trapped for an infinite time.

• For $T$ close to $T_c$, $\Sigma(T)$ vanishes linearly with $T - T_c$. At $T = T_c$ the number of local minima becomes non-extensive and a static transition of the 1RSB kind occurs.

As the system is cooled below $T_d$ a dynamical transition occurs. One can easily write some closed equation for two time quantities such as

$$C(t + t_w, t_w) = \frac{1}{N} \sum_i^N \langle \sigma_i(t + t_w)\sigma_i(t_w) \rangle,$$  \hspace{1cm} (5)

$$G(t + t_w, t_w) = \frac{1}{N} \sum_i^N \frac{\partial \langle \sigma_i(t + t_w) \rangle}{\partial h_i(t_w)}.$$  \hspace{1cm} (6)

If the system has reached equilibrium, the two time quantities depend only on the differences between the two times and are related by the equation

$$G(t) = -\frac{1}{T} \frac{\partial C(t)}{\partial t} \theta(t).$$ \hspace{1cm} (7)

These two properties, time-translation invariance (TTI) and the fluctuation-dissipation theorem (FDT) are properties of equilibrium dynamics.

Below $T_d$ the system has a regime of slow dynamics where, for large time differences $t \simeq t_w$, the relaxation of $C$ and $G$ is slower the larger $t_w$ is i.e. the older the system is. In this regime one can write the two-time quantities under the form
\[ C(t + t_w, t_w) = \tilde{C}\left(\frac{h(t + t_w)}{h(t)}\right) \quad \quad G(t + t_w, t_w) = \frac{1}{t + t_w} \tilde{G}\left(\frac{h(t + t_w)}{h(t)}\right), \quad (8) \]

Relation (8) is not valid under \( T_d \), but a generalized FDT can be written introducing a function \( X_{t_w}(C) \) by the relation

\[ G(t) = -\frac{X_{t_w}(C)}{T} \frac{\partial C(t)}{\partial t} \theta(t). \quad (9) \]

For large waiting times one has that \( X_{t_w}(C) \to X(C) \). The function \( X(C) \) generally characterizes the type of aging dynamics of the model. In models where \( T_d = T_c \) (i.e. \( p = 2 \)) one has that \( X(C) = x(q) \) while this equation does not hold in general though the two functions remain equal in structure \[16\]. The dynamical transition in mean field spin glasses is interpreted as due to the freezing of the system into one among the \( O(\exp N) \) metastable states, which for a long range model have an infinite lifetime in the \( N \to \infty \) limit.

The presence of metastable states with infinite time life is just an artifact of the mean field approximation and we do not expect \( T_d \) to mark an effective dynamical transition in a finite dimensional model. Correspondingly one should find \[18\] that the dynamical function \( X_{t_w}(C) \) becomes equal to the static \( x(q) = \int_0^q dq' P(q') \) in the limit of \( t, t_w \to \infty \) (in which \( C \to q \)) also for 1RSB models. Nevertheless, it should be still possible to observe a \( T_d \) higher then the critical temperature \( T_c \). In a finite-dimensional system that has a 1RSB mean field solution \( T_d \) should mark the onset of a two step relaxation process: the mean field-like relaxation of the system within a metastable state and the following decay of the metastable state due to activated processes.

3 The model

The model that we study in this work is a short range version of the Ising \( p \)-spin glass. We believe that for our purposes the Ising and spherical version of the \( p \)-spin are essentially equivalent.

The model is defined as follows. We consider a cubic tridimensional lattice of side \( L \). On each site of the lattice we put \( M \) Ising spins. The total number of spins is therefore \( N = M L^d \). Each spin interacts with \( M - 1 \) spins on its same site and with \( 2dM \) spins on its nearest-neighbour sites. The interactions \( J^{l_1, ..., l_p}_{i_1, ..., i_p} \) are quenched random variables.

The Hamiltonian of the model can be written as

\[ \mathcal{H}_p(\{\sigma\}) = \sum_{<i_1, ..., i_p>} \sum_{l_1, ..., l_p=1}^{L^d} J^{l_1, ..., l_p}_{i_1, ..., i_p} \sigma_{i_1} \cdots \sigma_{i_p} l_p. \quad (10) \]

By \( \sum_{<i_1, ..., i_p>} \) we mean the sum over all the sites of the lattice taking, for each couple of adjacent sites \( i \) and \( j \), \( p - k \) of the \( l_1, \cdots, l_p \) indexes equal to \( i \) and \( k \) indexes equal to \( j \). In other words, for each nearest neighbour sites \( i \) and \( j \), every interaction involves \( p - k \) spins of site \( i \) and \( k \) spins of site \( j \) with \( k \) running from zero to \( p \).
We consider discrete \((\pm 1)\) spin variables and we call \(\sigma_{i_l}^r\) the \(l^{th}\) spin of site \(i_r\) with \(l_r\) running from 1 to \(M\).

For large \(M\), each spin interacts with a large number of nearest neighbours and, in the limit \(M \to \infty\), the mean field approximation has to be exact. An analytical study of the model for large \(M\) has been performed in [11] where a Gaussian \(P(J_{i_1 \ldots i_p})\) is considered. The mean field solution of the model coincides with the solution of the long range Ising \(p\)-spin.

One could hope to peep into the finite-\(M\) case by perturbing around the \(M \to \infty\) limit. Calculating the \(O(1/M)\) corrections to the free energy and the Gaussian propagators one sees that a perturbative approach shows a transition which is very similar to the MF one, with a discontinuous \(q(x)\) and no diverging low-momentum static propagators. In the model that we simulated we chose the following distribution for the couplings

\[
P(J) = \frac{1}{2} \delta_{J,1} + \frac{1}{2} \delta_{J,-1}. \tag{11}\]

The fact that the distribution of the couplings is non-Gaussian should not be source of relevant differences from the analytical calculation. Any result in disagreement with the results of [11] should be imputed to finite dimensional effects which can not be reached with \(O(1/M)\) calculations.

Here we take \(M = 3\) and \(p=4\). Since \(p\) is even, the Hamiltonian is invariant for inversion of all the spins (\(\{\sigma_i^l\} \to \{-\sigma_i^l\}\)) and the \(P(q)\) is correspondingly symmetric, i.e. \(P(q) = P(-q)\).

As usual in spin glass simulations we consider two replicas (with the same configuration of disorder) of the system, with spin \(\{\sigma\}\) and \(\{\tau\}\) respectively, that evolve simultaneously and independently. We define

\[
Q \equiv \frac{1}{N} \sum_{i=1}^{L^3} Q_i \equiv \frac{1}{N} \sum_{i=1}^{L^3} \frac{1}{M} \sum_{l=1}^{M} \sigma_{i_l}^l \tau_{i_l}^l. \tag{12}\]

The order parameter probability distribution \(P(q)\) is then given by

\[
P(q) \equiv \langle \delta(q - Q) \rangle \tag{13}\]

where \(\langle \cdot \rangle\) means thermal average and \(\langle \cdot \rangle\) means average over disorder.

When looking at the out of equilibrium behaviour of the system it is useful to consider [17] the staggered magnetization

\[
m_s[h](t) = \frac{1}{L^3} \sum_{i=1}^{L^3} \langle \frac{1}{M} \sum_{l=1}^{M} \sigma_i^l(t) \rangle, \tag{14}\]

that is related to the response function \(G(t_1, t_2)\) by

\[
G(t_1, t_2) = \frac{\delta m_s[h](t_1)}{\delta h(t_2)}. \tag{15}\]

One has therefore

\[
m_s[h](t_1) = \int_{-\infty}^{t_1} dt_2 \frac{\delta m_s[h](t_1)}{\delta h(t_2)} = \int_{-\infty}^{t_1} dt_2 G(t_1, t_2) h(t_2) + O(h^2), \tag{16}\]

7
which is just the linear-response theorem.

By applying the generalized FDT relation (1) one obtains:

\[ m[h](t_1) \simeq \beta \int_{-\infty}^{t_1} dt' X[C(t_1, t_2)] \frac{\partial C(t_1, t_2)}{\partial t_2} h(t_2). \]  

(17)

If the small perturbing magnetic field is turned on at the time \( t_w \) to a constant time-independent value \( h_0 \) we get

\[ m_s[h](t_1) \simeq \beta h_0 \int_{t_1}^{t_2} dt' X[C(t_1, t_2)] \frac{\partial C(t_1, t_2)}{\partial t_2} = \beta h_0 S(C), \]

(18)

where we have used \( C(t_1, t_2)=1 \) for \( t_1 = t_2 \).

In the case of finite dimensional models, for large \( t_w \), \( t_1 = t + t_w \), one has \( C \to q \), \( X(C) \to x(q) \), where \( x(q) = \int_q^q dq' P(q') \). This means that the staggered magnetization measured by out of equilibrium simulations is related to static quantities and more precisely

\[ S(C) \to y(q) = \int_q^1 dq' x(q') \]

(19)

We are therefore allowed to confirm results on the equilibrium probability distribution of the overlaps \( P(q) \) by looking at the dynamical behaviour of large systems.

4 On the behaviour at the equilibrium

4.1 Simulations

In order to measure equilibrium quantities we use Parallel Tempering (PT) [19]. We consider size ranging from \( L=3 \) up to \( L=6 \) (\( N=648 \)), simulating contemporaneously two independent sets of \( n \) replicas that move between \( \beta_{\text{min}} = 0.14 \) and \( \beta_{\text{max}} = \beta_{\text{min}} + n\Delta \beta = 0.5 \) (i.e. down to \( T_{\text{min}}=2.0 \)), where \( \Delta \beta = 0.4 \) for \( L=3, 4 \) and \( \Delta \beta = 0.2 \) for \( L=5, 6 \). We perform \( 2^{18} \) PT steps for \( L=3, 2^{19} \) for \( L=4 \) and \( 2^{21} \) for \( L=5, 6 \), that means up to 2 millions of MC steps for each of the \( 2n=38 \) replicas.

Thermalization is checked in different ways:

- We measure all the relevant quantities during the whole run (in each \( 2^t - 2^{t+1} \) interval), looking at the convergence to equilibrium and checking that there are no shifts of the mean values in the last intervals. In particular, we do not find evident changes in the behaviour of \( P(q) \). The presented data are the ones collected in the last half of the run.

- We check that each replica moves several times from an extrema of the temperature range to the other and back.

- We evaluate the specific heat \( c \) both using \( c = \partial < e > / \partial T \) and using \( T^2 c = < e^2 > - < e >^2 \), checking the compatibility of the results (see [Fig. 1]).

Errors are estimated from the fluctuations between different disorder realizations. We consider 400 samples for \( L=3 \), 300 for \( L=4 \), 240 for \( L=5 \) and more than 100 for \( L=6 \).
4.2 Results on $\chi_{SG}$ and $P(q)$

We present in [Fig. 1] data on the energy and the specific heat as a function of $T$ for the different sizes considered. Finite size effects are quite evident for $L=3$ while the observed behaviours result very similar for larger $L$ values.

![Figure 1: Data on the energy density $e$ (left) and on the specific heat $c$ (right) as a function of $T$ for $L=3(\times)$, $4(\times)$, $5(\times)$ and $6(\square)$. Lines are only to join neighbouring points.](image)

The spin glass susceptibility $\chi_{SG} \equiv M L^3 \langle q^2 \rangle$ is plotted in [Fig. 2] for the different sizes considered. The obtained behaviour confirm [12] the presence of a non-zero $T_c$ thermodynamical transition which appears to be of second order. Data agree well [Fig. 3] with the finite size scaling law

$$\chi_{SG}(L, T)/L^{2-\eta} = \tilde{\chi}_{SG} \left( L^{1/\nu} (T - T_c) \right), \quad (20)$$

where we use $T_c \approx 2.6$, $\eta \approx 0$ and $\nu \approx 1$. The value of $\nu$ results slightly higher than the previously estimated $[12] \nu \approx 2/3$, this being probably due to some corrections to finite size scaling.

In [Fig. 4] we plot $P(q)$ for $L=5$ at different temperatures, from $T=3.33$ down to $T=2.0$. The behaviour emerging from these data results quite puzzling.

When approaching $T_c$, $P(q)$ becomes clearly non Gaussian but there is no evidence for the transition being discontinuous in the order parameter. Our data are compatible both with $q_1=O(T-T_c)$ at $T<T_c$ and with the possibility of a finite $q_1=O(1)$, hidden by finite size effect.

At lower temperatures the situation appears still less clear: From the mean field theory we expect only two possible values of the overlap, i.e. $q_0 = 0$ and $q_1$ which increases when lowering $T$, whereas we find a $P(q)$ which is clearly greater than zero in all the range $[-q_1, q_1]$ also at the lowest temperature considered $T=2.0$. Moreover we observe, as expected, the weight of the peak in $q_0$ to decrease when lowering $T$ but it widens, although never disappear completely.

We could suppose that these are finite size effects. It should also be noted that in the mean field spherical $p$-spin all the values of the overlap are allowed within metastable states [21] and the contribute of these states is expected to be negligible only at very large $N$. Nevertheless these effects do not appear to decrease as $L$ increases.
Figure 2: Data on the spin glass susceptibility $\chi_{SG}$ as a function of $T$ for $L=3(+)$, 4($\times$), 5($\ast$) and 6($\blacksquare$). Lines are only to join neighbouring points.

Figure 3: Data on the spin glass susceptibility $\chi_{SG}/L^2$ as a function of $(T-T_c)/L^{1/\nu}$ for $L=3(+)$, 4($\times$), 5($\ast$) and 6($\square$).
Figure 4: Data on $P(q)$ for $L=5$ (240 samples) at different temperatures. From left to right and top to bottom $T=3.33$, 2.94, 2.63, 2.38, 2.17 and 2.0.

Figure 5: Data on $P(q)$ for the different sizes. From left to right and top to bottom $L=3$, 4, 5 and 6.
Figure 6: Data on \( P(q) \) for \( L=6 \) (118 samples) at the lowest temperature considered \( T = 2.0 \) as obtained in the last half of the run (right) and in the previous interval (i.e. in the previous \( 2^{20} - 2^{19} \) PT steps).

As it can be seen from [Fig. 5], where we present data on \( P(q) \) at \( T=2.0 \) for the considered sizes, the minimum value \( P_{\text{min}} = \min_{q \in [-q_1, q_1]} P(q) \) for \( L=3 \) \((N=81)\) is compatible within the errors with the one for \( L=6 \) \((N=648)\). Moreover the broadening of the peak in \( q_0 \) when considering larger sizes is very evident if we compare data for \( L=3 \) with the ones for \( L=5 \).

The comparison between the \( L=5 \) and \( L=6 \) data on \( P(q) \) results puzzling since the weight of the peak in \( q_0 \) seems to be larger in the last case. On the other hand it is well known that a correct estimation of \( P(0) \) in spin glass simulations requires great care since the possible presence of non well thermalized samples causes the overestimation of this value.

In order to clarify this point we plot in [Fig. 6] \( P(q) \) for \( L=6 \) at \( T=2.0 \) in the last half of the run (the same data that in [Fig. 5]) and in the previous interval (i.e. in the previous \( 2^{20} - 2^{19} \) PT steps). Although data are compatible within the errors, the shift of the peak in \( q_0 \) is quite evident (this is an effect that we do not observe in \( L=5 \) data) and it shows that some of the samples are still not perfectly equilibrated at the beginning of the last half of the run. We are therefore suspicious that \( 2^{23} \) PT steps would be needed to be sure of achieving a complete thermalization for \( L=6 \) down to \( T=2.0 \), which means unfortunately too much CPU time.

If the peak in \( q_0 \) would disappear completely when considering larger size, the \( P(q) \) would display a FRSB-like behaviour at low temperatures, i.e. two peaks in \( \pm q_1 \) separated by a continuous plateau. Nevertheless, by looking carefully both to \( L=5 \) and \( L=6 \) data at low temperatures and to the previous [Fig. 5], we note that the broadening of this peak is related to the appearance of smaller, not well pronounced peaks near \( q_0 \) and that the behaviour of the \( P(q) \) near and below \( T_c \) results very different from the one usually encountered in short range models with FRSB [21].

To emphasize the last observation, we present in [Fig. 7] data on the cumulant

\[
g(T) = \frac{1}{2} \left( 3 - \frac{\langle q^4 \rangle}{\langle q^2 \rangle^2} \right). \tag{21}
\]

This is the well known dimensionless parameter usually successful for evaluating \( T_c \), since \( g(T) \) should go to zero above \( T_c \) in the thermodynamic limit and the curves for different values of
Figure 7: Data on $g(T)$ for $L=5$ (240 samples) at different temperatures. From left to right and top to bottom $T=3.33, 2.94, 2.63, 2.38, 2.17$ and $2.0$.

$N$ should cross at the critical temperature because of finite size scaling. In the FRSB mean field models as well as in their short range versions (EA models) $g(T)$ for finite $N$ is an always positive function of $T$ that increases quite regularly when lowering the temperature. The behaviour displayed in [Fig. 7] results therefore in evident disagreement with the one expected in the usual FRSB case: we find a $g(T)$ which is a non monotonic function of $T$, negative on a large part of the range of temperatures considered. This accounts for the fact that the function $P(q)$ develops non-Gaussian tails in a range of temperatures above $T_c$ detecting the presence of non perturbative effects (see the related discussion in the conclusions). The shown data correspond to $L=5$ but the behaviour is qualitatively similar for the other $L$ values that we have considered and it suggests that this model belongs to a different universality class from the EA spin glass one.

In conclusion, more extensive simulations are necessary to achieve a better understanding of the short range $p$-spin glass. Nevertheless it seems quite evident from our data that we are looking at a model characterized by a $P(q)$ that is in disagreement with the one of 1RSB mean field models but that appears also very different from the one usually encountered in FRSB models. This is a quite new result that may have interesting physical interpretations as we will discuss in the following.

5 On the dynamical behaviour
5.1 The approach to the equilibrium

We have already pointed out that the infinite time life of metastable states is an artifact of mean field theory. We therefore do not expect to find a dynamical transition at $T_d > T_c$ in a short range system. On the other hand it should be possible to observe a “reminiscence” of the mean field $T_d > T_c$ in the 1RSB case by looking at the energy density relaxation when the system, starting from a random configuration, is quenched abruptly (i.e. infinite cooling rate) to a low $T$ value.

Recent numerical results on a glass-forming system \[8, 22\] seem to show that $T_d$ is identifiable in short-range models as the temperature below which the energy density $e(t)$ displays a two step relaxation. The first step corresponds to the relaxation of the system to some metastable states with a mean field like behaviour \[12\], $e(t) \propto t^{-\alpha}$ where $\alpha$ is weakly depending on $T$. The second one, that happens on a remarkably larger time scale, is due to the slow decay of metastable states by activated processes.

We study the relaxation behaviour of $e(t)$ by considering a non small size $L=25$. Starting from a random initial configuration the system is quenched to the final temperature and it evolves by Monte Carlo, each spin being suggested to flip in one MC step. Presented data are averaged over two independent dynamics.

![Figure 8: Data on $e$ as a function of $y = t^{-d_e/z(T)}$ at different temperatures. From left to right and top to bottom, $T=2.60(+) , 2.3(\times), 1.95(\ast)$ and $1.3(\square)$, where $y=t^{-0.20}, t^{-0.17}, t^{-0.15}$ and $t^{-0.10}$ respectively.](image-url)

The energy density $e$ is presented in [Fig. 8] as a function of $y = t^{-\alpha_e(T)}$ at the different temperatures considered $T=2.60 (\simeq T_c)$, 2.30, 1.95 and 1.30. These data are well consistent with a linear behaviour of $e$ as a function of $y$ also at large times (small $y$), i.e. there is no evidence for a two step relaxation. Moreover at the higher temperatures we have considered the system seems near to the equilibrium at the end of the time window and correspondingly...
the values of \( e \) result compatible with the equilibrium ones obtained from the previously shown data on smaller systems.

The observed behaviour gives evidence for the dynamical critical temperature coinciding with the statical one, \( T_d = T_c \), as it happens in models with FRSB.

Since we are looking at a second order transition, \( \alpha \) is related to the dynamical critical exponent \( z \) by \( \alpha e(T) = d - 1/\nu \). We get \( \alpha e \approx 0.2 \) at \( T = 2.6 \approx T_c \) that agrees well with the previous estimates \([12]\) \( \nu \approx 2/3 \), \( z(T_c) \approx 7 \). Our statistics is inadequate to give meaningful results on the behaviour of \( z(T) \), which appears however definitely dependent on \( T \), the obtained estimation being consistent with \( z(T) = z(T_c) T_c/T \).

To conclude this section we present in [Fig. 9] data on

\[
C(2t, t) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{1}{M} \sum_{l=1}^{M} \sigma_{i}^{l}(2t)\sigma_{i}^{l}(t) \right) 
\]

(22)

plotted as a function of \( y = t^{-\alpha q c} \), where \( \alpha q c = \alpha q (T \approx T_c) \approx 0.06 \).

At \( T = 2.6 \approx T_c \) the observed behaviour is consistent with \( C \) going to zero linearly in \( t^{-\alpha q c} \). By scaling laws one has \( \alpha q c = d_q/z(T_c) \), where \( d_q = (d - 2 + \eta)/2 \). We note that \( \alpha q c \approx 0.06 \) agrees with \( \eta \approx 0 \), \( z(T_c) \approx 7 \). Our statistics results inadequate to fit data at lower temperatures where the behaviour results consistent with \( C \) going to a non-zero value for \( t \to \infty \) at \( T < T_c \).

![Figure 9: Data on \( C(2t, t) \) as a function of \( y = t^{-d q/z(T_c)} = t^{-0.06} \) at \( T=2.6(+) \), 2.3(\( \times \)), 1.95(\( * \)) and 1.3(\( \square \)).](image-url)
5.2 Aging and generalized FDT

The data presented in this section are obtained by MC simulations on a $L=16$ system at $T=2.0$, i.e. well below the critical temperature. We average over 50 different dynamics (initial conditions and realizations of the thermal noise). Starting from a random configuration, the system is quenched abruptly to the final temperature. After $t_w$ steps we apply a small perturbing magnetic field $\delta h = h_0 = 0.4$, measuring the two times correlation function

$$C(t + t_w, t_w) = \langle \frac{1}{M} \sum_{l=1}^{M} \sigma_i \sigma_i^l(t + t_w) \rangle$$

and the staggered magnetization

$$m_s[h](t + t_w) = \frac{1}{N} \sum_{i=1}^{N} \langle \frac{1}{M} \sum_{l=1}^{M} \sigma_i \rangle.$$  

The behaviour of $C(t + t_w, t_w)$ for different values of $t_w$ is shown in [Fig. 10] on the left. On the right we plot the same data as function of $t/t_w$. The hypothesis of simple aging, i.e. $C(t + t_w, t_w) = \tilde{C}(t/t_w)$, seems to be not well verified.

![Figure 10: Data on $C(t + t_w, t_w)$ plotted as function of $t$ (left) and as function of $t/t_w$ (right) for $t_w = 2^6$, $2^8$, $2^{10}$, $2^{11}$, $2^{12}$, $2^{13}$, and $2^{14}$.](image)

In [Fig. 11] we plot $m_s[h](t + t_w)/(\beta h_0)$ as a function of $C(t + t_w, t_w)$ for different values of $t_w$. Here the expected scaling is quite well satisfied and we are therefore allowed to take the large times behaviour of this quantity as an estimation for $S(C)$. The behaviour of $m_s[h](t + t_w)/(\beta h_0)$ at $t_w = 2^{17}$ (i.e. the largest value considered) is presented in [Fig. 12] together with the estimation of $y(q) = \int_0^1 dq' \int_0^{q'} dq'' P(q'')$ as obtained by the $L=5$ data on $P(q)$. As expected, the dynamical function $S(C)$ results perfectly compatible with the statical one $y(q)$. This dynamical quantity, obtained by simulating a non small system, gives further evidence that the model does not behave like MF 1RSB spin glasses.

We have shown in the figure the line corresponding to $1 - C$ just to emphasize the small $t$ region where FDT is satisfied. The $q_1$ value is evaluable as the one where $y$ begins to move
Figure 11: Data on $m_s[h](t+t_w)/(\beta h_0)$ plotted as function of $C(t+t_w, t_w)$ for $t_w=2^6(\times), 2^8(\times), 2^{10}(\ast), 2^{11}(\square), 2^{12}(\bigtriangleup), 2^{13}(\bigcirc), 2^{14}(\bullet)$.

Figure 12: Data obtained from the dynamics on $m_s[h](t+t_w)/(\beta h_0)$ plotted as function of $C(t+t_w, t_w)$ at $t_w=2^{17}(\times)$ compared with the behaviour of $y(q)$ as obtained from the $P(q)$ for $L=5$ (the line with error bars). The $\ast$ represents a dynamical estimation for $\lim_{C\to0} S(C)$ as obtained by a simulation in which the magnetic field is switched on from the beginning. We also plot $1-C$ (see the text).
away from this line. In mean field 1RSB models we observe a straight line for \( y \) going from \( q_1 \) to 0 (the dynamical function \( S(C) \) showing the same structure than the statical one):

\[
y(q) = \begin{cases} 
(1 - m)(q_1 - q) + (1 - q_1) & \text{for } q \leq q_1 \\
1 - q & \text{for } q \geq q_1
\end{cases}
\]  
(25)

This behaviour has been recently observed in simulations of structural glasses [7], by defining appropriately the correlation function \( C \) and the response function to small perturbations \( R \).

In the case of our model, instead of been in agreement with (25), \( S(C) \) (we dynamically estimate \( S(0) \) extrapolating data obtained by a simulation in which \( h \) has been switched on from the beginning) results more similar to the one observable in FRSB models [17, 23], confirming the results on the equilibrium probability distribution \( P(q) \) at low temperatures.

6 Discussion and conclusions

Summing up our main results:

- The transition appears to be of second order, characterized by a diverging correlation length for \( T \to T_c \simeq 2.6 \). Our estimations for the critical exponents agree with the ones previously obtained [12] \( \nu \simeq 2/3, \eta \simeq 0, z \simeq 7 \).

- There is no evidence for the dynamical critical temperature \( T_d \) being greater then the statical one, where in finite dimensional models that are 1RSB in mean field \( T_d > T_c \) should mark the onset of two steps relaxation processes.

- The distribution probability of the overlaps \( P(q) \) results non trivial at low temperature but its behaviour is very different from the one of mean field 1RSB models.

- Well below \( T_c \), we find a \( P(q) \) still definitely non-zero on the whole interval \([-q_1, q_1]\). This result is confirmed by out of equilibrium simulations on a quite larger lattice (i.e. by the behaviour of \( S(C) \) which is related to \( P(q) \) by the generalized FDT relation).

- The behaviour of \( P(q) \) seems nevertheless also not compatible with the one usually encountered in FRSB models, this resulting well evident if one looks at the cumulant \( g(T) \).

Our possible interpretation of this phenomenology is the following. In this model the disorder is not space-invariant. In each particular sample there will be a finite density of regions which are more likely than the rest of the system to freeze into a SG phase. Hence when \( T \to T_c \) there is a non-zero probability to find a region of space where the system is in the 1RSB phase. The typical size of these regions will diverge when \( T \) approaches \( T_c \) since the system freezes at the critical temperature. In these regions the spins are very correlated and one can formally divide the total high temperature spin glass susceptibility into the contribution of bubbles of frozen spins and the contribution of the rest of the system. We write

\[
\chi_{SG} = \chi_B + \chi_R
\]  
(26)
where $B$ stands for “bubbles” and $R$ for “rest”. So, for $T$ approaching $T_c$ from above one has

$$\chi_B \propto (T - T_c)^{-\gamma} \quad \chi_R = O(1)$$

(27)

It is important to note that this kind of transition, at least from this analytical point of view, is very different from an ordinary second order transition in mean field, where a zero mass mode on the mean field solution causes diverging correlations. Here the high temperature solution is stable and non-perturbative effects dominate the approach to the transition. Within the bubbles the transition can still be similar to the MF 1RSB. It is the weight of the bubbles that grows continuously and diverges when $T \to T_c$.

It is possible that a similar phenomenon is responsible for the fact that the function $P(q)$ does not tend to the sum of two delta functions at $T_c$ (opposite to what happens in mean field theory). This point deserves a more careful study.

Acknowledgments

We are happy to thank Felix Ritort for a careful reading of the manuscript and for fruitful related discussions.

References

[1] M. Mezard, G. Parisi, and M.A. Virasoro, *Spin Glass Theory and Beyond*, World Scientific (1987).

[2] T.R. Kirkpatrick and D. Thirumalai, Phys. Rev. B 36, 5388 (1987); T.R. Kirkpatrick and P. G. Wolynes, Phys. Rev. B 36, 8552 (1987); a review of the results of these authors and further references can be found in T.R. Kirkpatrick and D. Thirumalai Transp. Theory and Stat. Phys. 24, 927 (1995).

[3] For a review see, W. Gotze, *Liquid, Freezing and the Glass Transition*, Les Houches (1989), J. P. Hansen, D. Levesque, J. Zinn-Justin editors, North Holland; C. A. Angell, Science 267, 1924 (1995).

[4] G. Parisi, *On the Replica Approach to Glasses* Proceeding of the ACS meeting at Orlando.

[5] G. Parisi, *New Ideas in Glass Transitions* Proceedings of International workshop on The Morphology and Kinetics of Phase Separating Complex Fluids (Messina, June 1997).

[6] G. Parisi, J. Phys. A: Math. Gen. 30, 8523 (1997).

[7] G. Parisi, Phys. Rev. Lett. 79, 3660 (1997).

[8] B. Coluzzi and G. Parisi, *On the Approach to the Equilibrium and the Equilibrium Properties of a Glass-Forming Model*, J. Phys. A: Math. Gen. (in press).
[9] M. Cardenas, S. Franz and G. Parisi, J. Phys. A: Math. Gen. 31, L163 (1998).

[10] M. Cardenas, S. Franz and G. Parisi, *Constrained Boltzmann-Gibbs measures and effective potential for glasses in hypernetted chain approximation and numerical simulations*, preprint cond-mat/9801153.

[11] M. Campellone, G. Parisi and P. Ranieri, Finite dimensional corrections to mean-field in a short range p-spin glassy model, to be published

[12] S. Franz and G. Parisi, *work in progress*.

[13] E. Marinari, C. Naitza, F. Zuliani, G. Parisi, M. Picco and F. Ritort, *A general method to determine replica symmetry breaking transitions*, preprint cond-mat/9802309.

[14] G. Parisi, M. Picco and F. Ritort, *work in progress*.

[15] L. Cugliandolo and J. Kurchan, Phys. Rev. Lett. 71, 173 (1993).

[16] L. Cugliandolo and J. Kurchan, J. Phys. A: Math. Gen. 27, 5749 (1994).

[17] S. Franz and H. Rieger, J.Stat.Phys. 79, 749 (1995).

[18] S. Franz, M. Mézard, G. Parisi and L. Peliti, *Measuring equilibrium properties in aging systems*, preprint cond-mat/9803108.

[19] M.C. Tesi, J. van Rensburg, E. Orlandini and S.G. Whillington, J. Stat. Phys. 82, 155 (1996).

[20] A. Cavagna, I. Giardina and G. Parisi, J. Phys. A: Math. Gen. 31, 3115 (1998).

[21] J. C. Ciria, G. Parisi and F. Ritort, J. Phys. A: Math. Gen. 26, 6731 (1993).

[22] B. Coluzzi, G. Parisi and F. Ricci-Tersenghi, *work in progress*.

[23] E. Marinari, G. Parisi, F. Ricci-Tersenghi and J.J. Ruiz-Lorenzo, J. Phys. A: Math and Gen. 31, 2611 (1998).