ELSEVIER

Physica A 286 (2000) 1–9

PHYSICA A

www.elsevier.com/locate/physa

Complexity and line of critical points in a short-range spin-glass model

M. Campellone[a,*], F. Ritort[b]

[a] Dipartimento di Fisica and Sezione INFN, Università di Roma "La Sapienza", Piazzale A. Moro 2, 00185 Rome, Italy

[b] Departament de Fisica Fonamental, Facultat de Fisica, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

Received 20 December 1999

Abstract

We investigate the critical behavior of a three-dimensional short-range spin-glass model in the presence of an external field ε conjugated to the Edwards–Anderson order parameter. In the mean-field approximation this model is described by the Adam–Gibbs–DiMarzio approach for the glass transition. By Monte Carlo numerical simulations we find indications for the existence of a line of critical points in the plane (ε, T) which separates two paramagnetic phases. Although we may not exclude the possibility that this line is a crossover behavior, its presence is direct consequence of the large degeneracy of metastable states present in the system and its character reminiscent of the first-order phase transition present in the mean-field limit. We propose a scenario for the spin-glass transition at $\varepsilon = 0$, driven by a spinodal point present above T_c, which induces strong metastability through Griffiths singularities effects and induces the absence of a two-step shape relaxation curve characteristic of glasses.

PACS: 05.50.+q; 75.50.Lk; 64.60.Cn

Keywords: Disordered systems; Glass transitions; Spin Glasses

Among all different approaches to understand the glass transition the thermodynamic theory of Adam–Gibbs–Di Marzio (AGM) has deserved a lot of interest during the last decades [1,2]. The AGM theory predicts the occurrence, at a Kauzman temperature T_K, of a second-order phase transition for the undercooled liquid where the configurational entropy (also called complexity) vanishes. The validity of the AGM theory for real glasses has never been demonstrated so the correct description of the glass transition

* Corresponding author.

E-mail addresses: matteo.campellone@roma1.infn.it (M. Campellone), ritort@ffn.ub.es (F. Ritort)

0378-4371/00/$ - see front matter
PII: S0378-4371(00)00060-1

still remains open [3]. An alternative dynamical approach (mode-coupling theory hereafter referred as MCT, for review see Ref. [4]) was proposed to describe relaxational processes in the undercooled liquid regime, experimentally observed in scattering and dielectric measurements.

Quite recently, it has been realized that spin glasses are models which account for both the thermodynamic (AGM) and the dynamical (MCT) approaches [5,6]. Although spin glasses are models with quenched disorder (and structural glasses are not) this is not an essential difference because the existence of a crystal phase in structural glasses has no dramatic effect in the dynamics of the (disordered) undercooled liquid phase. Unfortunately, up to now this connection between spin glasses and glasses remains only at the mean-field level and it is not clear what happens if one considers short-range interactions. In fact, concepts such as complexity in AGM or the ergodicity parameter in ideal MCT are originally mean field and it is not clear their relevance in short-ranged realistic systems.

It has been suggested [7–11] that the effect of the complexity could be observed through numerical simulations in a generic glassy system coupling two replicas by introducing a term in the Hamiltonian of the type $-\varepsilon q$ (ε being the *conjugate* field of the order parameter q which is the overlap between the configurations of the two replicas, for introductory text see Refs. [12–14]). The study of an exactly solvable spin-glass model has revealed the existence of a first-order transition line $T_c(\varepsilon)$ with a critical end-point [7,8]. This result is a consequence of the fact that the glass transition for $\varepsilon = 0$ (where the complexity vanishes) is a first-order phase transition (in the sense that the order parameter q is discontinuous) and the point $T_c = T_c(\varepsilon = 0)$ is a tricritical point. Again, this result has been obtained within the mean-field approximation and it is unclear that to what extent this result is valid in a finite-dimensional model. Recent numerical simulations on a short-range version of p-spin Ising spin glass [15–19] have shown that the mean-field discontinuous transition becomes continuous in finite dimensions. So the first-order character of the transition predicted in mean-field theory dramatically changes in finite dimensions. Nevertheless, in this work we would like to show that some features of the mean-field approximation, at least in the way of a crossover behavior, survive in finite dimensions. This allows to interpret our findings in terms of a picture for a continuous spin-glass transition induced by the strong metastability and driven by the collapse of the complexity or configurational entropy similar to what happens in structural glasses. Furthermore, our results point in the direction that disordered systems in three dimensions are very well described by a line of critical points (characteristic of systems at their lower critical dimension) in agreement with recent numerical simulations in the Edwards–Anderson model in three dimensions [20]. Nevertheless, we must stress that, from the point of view of numerical simulations, it remains unclear whether the critical line observed is merely a crossover regime (in the sense that this line will eventually disappear in the $L \to \infty$ limit). Also, in this case, the study of a crossover behavior is relevant because it should induce strong non-equilibrium effects. Let us note in passing that the same question (i.e., to discern between a crossover behavior and a real transition) also arises in structural glasses when trying to understand whether the Kauzman singularity indeed exists beyond mean field.

We shall consider a recently introduced short-range p-spin glass model [15–19] which is defined on a d-dimensional hypercubic lattice. On each site of the lattice there are M spins interacting with the following Hamiltonian

$$\mathscr{H}_p(\{\sigma\}) = -\sum_{\langle i_1,\dots,i_p\rangle}^{L^d} \sum_{l_1,\dots,l_p=1}^{M} J_{i_1\dots i_p}^{l_1\dots l_p} \sigma_{i_1}^{l_1}\cdots\sigma_{i_p}^{l_p} . \tag{1}$$

By $\sum_{\langle i_1,\dots,i_p\rangle}^{L^d}$ we sum over all sites of the lattice all possible groups of p spins that can be formed between spins on the same site and spins of adjacent sites. In this work, we consider Ising spin variables. By $\sigma_{i_r}^{l_r}$ we denote the l_r^{th} spin of site i_r with the index l_r running from 1 to M. For $p=2$ Eq. (1) corresponds to the Edwards–Anderson model. Although this model may seem quite artificial it has the advantage of including multispin interactions in a lattice without introducing new symmetries which may change the degeneracy of the ground state [21].

Here we consider two identical coupled models (each defined through Eq. (1)) via the following Hamiltonian

$$\mathscr{H}_p^2(\{\sigma\},\{\tau\}) = \mathscr{H}_p(\{\sigma\}) + \mathscr{H}_p(\{\tau\}) - \varepsilon V q , \tag{2}$$

where $V=L^3$ is the volume and $Vq=\sum_{i=1}^{V}\sigma_i\tau_i$ defines the order parameter. Note that, for two coupled systems the order parameter space is larger than we suppose here. Actually, a complete study of all possible phases requires the knowledge of the overlaps $\langle\sigma_i^a\sigma_i^b\rangle$ as well as $\langle\tau_i^a\tau_i^b\rangle$ where a,b stand for replica indices in the usual statistical mechanics approach to disordered systems [12–14]. Mezard [11] has presented a detailed study of all the possible phases of the mean-field p-spin model with two coupled replicas. For small values of ε there is a transition between a correlated glass phase and an uncorrelated liquid while for larger values of ε the transition occurs to a correlated liquid phase (also called molecular liquid). Actually, for $\varepsilon\to\infty$ there must be a transition at a temperature $2T_c(\varepsilon=0)$ because in that case $\sigma_i=\tau_i$. Here we will analyze the case of a small value of the coupling ε, well below the temperature where a transition to a molecular liquid occurs. Because the $\varepsilon=0$ transition in this model is continuous we naively expect that (similarly to what happens in the Edwards–Anderson model) there is no phase transition for $\varepsilon\neq 0$. In mean-field models with a one-step replica broken phase there is a transition line which separates two paramagnetic phases with a finite latent heat (which vanishes at the critical endpoint) [7–11]. The two possible phases (glass and liquid) are depicted in Fig. 1. The figure is a simplified representation of the different phases of the model where the molecular liquid has not been included (this would require to introduce more order parameters enlarging the dimensionality of the phase diagram). [1] The Edwards–Anderson order parameter q_{EA} (defined as the infinite-time limit of the equilibrium autocorrelation function [12–14])

[1] We are grateful to M. Mézard for calling our attention on this point.

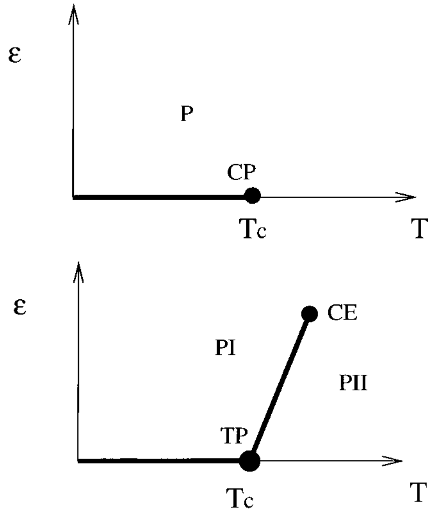

Fig. 1. ε–T phase diagram for the Edwards–Anderson model (above) and the short-range p-spin model (below). In the former case there is a single paramagnetic phase, in the latter two different paramagnetic phases divided by a critical line which connects a tricritical point (TCP) and a critical endpoint (CE) (for p even the line $TP - CE$ exists also for $\varepsilon < 0$).

displays a finite jump across the line $T_c(\varepsilon)$ which vanishes at the critical endpoint. Here we find strong indications, through Monte Carlo simulations, that this first-order line $T_c(\varepsilon)$ persists in finite dimensions (at least as a crossover behavior) but becomes a line of *critical points*. So, in finite dimensions the first-order line becomes continuous (i.e., $q_{\rm EA}$ is continuous when crossing the transition line and there is no latent heat), the critical endpoint displaying a higher-order singularity.

In this paper we will focus our research of Eq. (1) for case $M = 3$, $p = 4$ in $D = 3$. Measurements of the spin-glass susceptibility for Eq. (1) show that this model has a continuous finite-temperature phase transition at $T_c \simeq 2.6$ with a divergent spin-glass susceptibility and a small negative specific heat exponent [15–17]. To evidenciate a phase transition for finite ε which separates two different paramagnetic phases we have done a detailed Monte Carlo study of the Binder parameter as a function of both the coupling ε and the temperature in the paramagnetic region. [2] The Binder parameter is usually defined through the relation,

$$g(\varepsilon, T) = \frac{1}{2}\left(3 - \frac{\overline{(q - \langle q\rangle)^4}}{\overline{((q - \langle q\rangle)^2)}^2}\right), \tag{3}$$

where $\langle \cdots \rangle$ stands for statistical average and $\overline{(\cdot)}$ for disorder average. Concerning the Binder parameter we expect it should vanish everywhere in both paramagnetic phases

[2] Monte Carlo simulations use the parallel tempering algorithm with 14 temperatures in the temperature range 3.0–5. We simulated four different lattice sizes $L = 3, 4, 5, 6$ with 100, 100, 100, 50 samples and $2^{14}, 2^{17}, 2^{19}, 2^{20}$ thermalization steps, respectively. Statistics was collected in a time window four times the previous thermalization times.

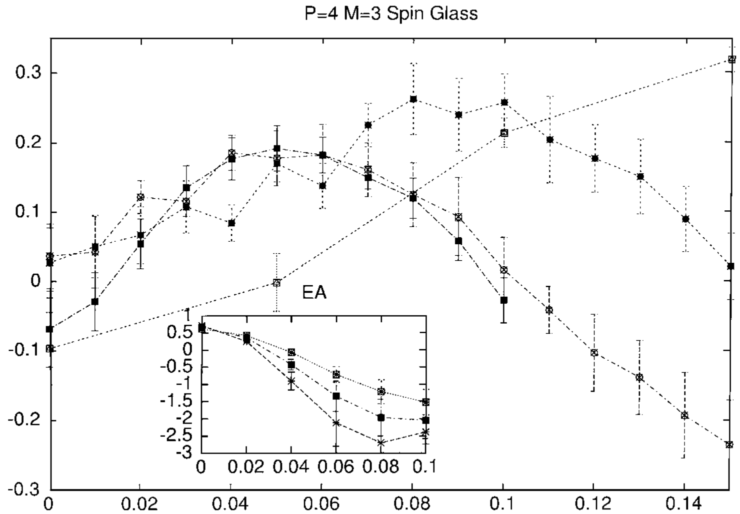

Fig. 2. Binder parameter as a function of ε at temperature $T = 3.2$ for different sizes ($L = 3$ empty squares, $L = 4$ filled circles, $L = 5$ empty circles, $L = 6$ filled squares). The same plot for the Edwards–Anderson model (inset) with $T = 1.3, 1.4, 1.5$ ($T_c \simeq 1.2$ [22]) shows a completely different behavior compared to the $p = 4$ model.

except at the critical line where it should be finite. So, if we fix ε (or, equivalently the temperature) and vary the temperature (equivalently ε) we expect the presence of a maximum approximately located on the transition line at a temperature $T_c(L, \varepsilon)$. The results for $g(\varepsilon, T)$ are shown in Fig. 2 for $T = 3.2$ and different sizes. Note that the Binder parameter shows a maximum located at $\varepsilon = 0.05$. As a comparison we also show simulations for the Edwards–Anderson model in three dimensions above T_c by coupling two replicas which evidenciate the absence of a maximum in that case. So the presence of a maximum in $g(\varepsilon, T)$ already for small sizes is a main feature of this model. For $L = 3, 4, 5$ finite-size corrections appear to be quite strong (this was already observed in Refs. [15–17] by measuring the $P(q)$) and the position of the maximum of the Binder parameter as well as its value both shift with L. Nevertheless, the maximum of the Binder parameter for $L = 6$ superimposes with the maximum for $L = 5$ and the Binder parameter, as L increases, goes to zero far from the maximum. This result indicates the presence of a critical line which separates two paramagnetic phases. A more stringent test of this result requires simulating larger sizes than those we did. Unfortunately, for $L = 7$ the thermalization time is much larger than what we can afford with the present numerical methods. Actually, a test of the needed thermalization time shows that it grows dramatically with L and for $L = 7$ and $T = 3.2$ this may be larger than several hundreds of million of Msteps for a nonvanishing fraction of disorder realizations. The impossibility to study larger sizes does not allow us to exclude the possibility of a crossover behavior. As we will discuss later, this strong size-dependent thermalization time is consequence of the large metastability and the highly corrugated landscape

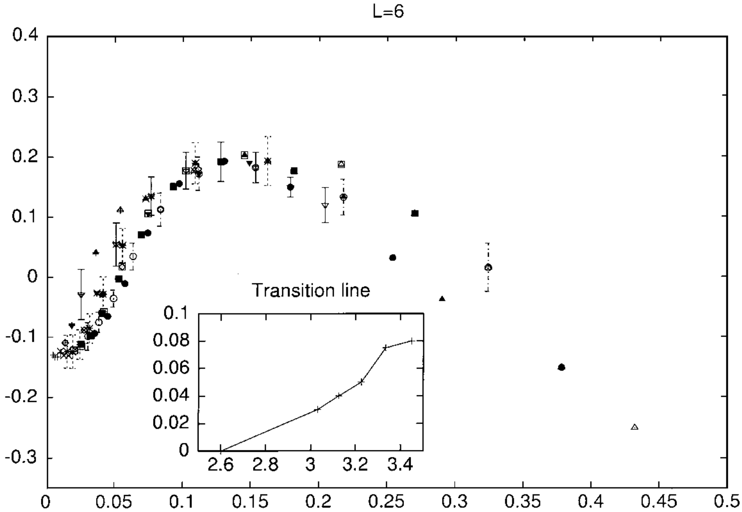

Fig. 3. Binder parameter plotted as a function of $\varepsilon(T-2.6)^{-2}$ in the range $0.01 \leqslant \varepsilon \leqslant 0.09$, $3.0 \leqslant T \leqslant 4.0$ for $L=6$. In the inset we show the estimated critical line (see the text) compared to the points for $L=5,6$ where appears a maximum of g in the plane (εT).

characteristic of this model which induces the existence of this critical line (which, on the other hand, is not found in the Edwards–Anderson model). Note that the fact that the maximum value of g along the critical line is smaller than one (approximately 0.2) is an indication that the transition should be continuous in q (if there were a finite jump in q the maximum value of g should be unity). Moreover, our data do not show any indication of a jump in the value $q(\varepsilon)$ as a function of the temperature (or $q(T)$ as a function of ε) in the vicinity of the region where there is the maximum of g.

In what follows we try to estimate the shape of this critical line using finite-size scaling techniques. A detailed investigation of its shape as well as its critical exponents is presently out of reach due to the smallness of the sizes studied. Still we can approximately determine them. Let us suppose (as data of Fig. 2 suggest) that there is a critical line $\varepsilon \sim C(T-T_c)^{\lambda}$ where $C, \lambda > 0$ and $T_c \simeq 2.60$. Assuming the validity of the scaling hypothesis we may write $g(T,\varepsilon) \equiv \hat{g}(\varepsilon(T-T_c)^{-\lambda})$. In Fig. 3 we plot the scaling behavior within the scaling region for different values of T and ε for the largest size $L=6$. The scaling is quite good and proves two results: (1) The position of the maximum stays along a well-defined line in the (ε, T) plane and (2) The value of the maximum of g is the same everywhere along that line. A good collapse of data is obtained with an exponent $\lambda \simeq 2$. The position of the maximum of the scaled data yields a value of $C \simeq 0.17$ and $g_{\max} \simeq 0.2$. This value is universal along the critical line and approximately coincides with the value of the Binder parameter at the tricritical point [15–17]. Although we expect that the critical line will have some L dependence, very similar results obtained for $L=5$ indicate that our estimate of the critical line for $L=6$ is reasonable. Our results confirm the theoretical scenario presented in Ref. [11]

showing that the shape of the critical line for small values of ε is not far from the mean-field result.

Now, we discuss the physical interpretation of this critical line. As mentioned in the introduction, whatever the nature of this line (critical or crossover) its presence is reminiscent of the first-order character of the transition in the mean-field approximation. Furthermore, the strong metastability which induces a hard thermalization is related to the properties of the metastable basins which are narrow and stable very much alike to what is found in the random-energy model of Derrida [23]. Again this is reminiscent of the first-order character of the transition in the mean-field limit. In mean-field theory (AGM or ideal MCT) metastable states have an infinite lifetime so there are infinitely large barriers which separate them. This is the reason why in mean-field theory ergodicity already breaks at the mode-coupling (also called dynamical) temperature. In short-ranged systems or real glasses metastable states decay by nucleation processes so ergodicity is always restored. A typical feature of the ideal MCT singularity is the characteristic two-step relaxational decay in correlation functions, the so-called α and β processes. In ideal MCT the typical relaxation time associated to the α process diverges at T_d and the ergodicity parameter jumps discontinuously at T_d. An accurate study of correlation functions reveals that the two-step characteristic relaxation curve is absent in the present model (1) [15–19]. The absence of a plateau in these curves indicate that do not exist two well-separated time-scales (α and β), like in generic glass-forming liquids, but a continuous hierarchy of time scales of nucleation processes. We interpret this result as consequence of the continuous nature of the transition everywhere in the critical line ε–T. A possible scenario for the potential function [24] for this type of transition is depicted in Fig. 4. Although this figure must be interpreted with caution it is indicative of how the present behavior, being critical or crossover, should compare with the mean-field prediction. In the figure we show that there is not a typical time scale for nucleation processes (where a small excited droplet or bubble decays from $q = q_{\rm EA}$ to $q = 0$) and the potential around the secondary minimum $q = q_{\rm EA}$ is marginally stable. Across the critical line the Edwards–Anderson parameter $q_{\rm EA}$ is continuous but $dq_{\rm EA}/{\rm d}\varepsilon$ is discontinuous, the potential being completely flat in q. Note that at $T = T_c, \varepsilon = 0$ where the complexity vanishes, the Edwards–Anderson parameter is also continuous in agreement with the absence of the two-step relaxation in this model. The complexity in this model is defined by the height of the secondary saddle point which moves towards $q = 0$ for $T = T_c$. The present scenario is very different to that found in the Edwards–Anderson model in finite dimensions where no additional spinodal point (apart from the paramagnetic one $q = 0$) has been found above T_c. Concerning dynamical processes and thermalization effects this model behaves also quite differently. Spatial regions may be frozen if their local temperature (measured always respect to the intensity of the local interaction) is low enough for nucleation processes to decay very slowly. This is apparent from Fig. 4 where the secondary saddle point may become a stable minima in certain Griffiths regions. This effect has been observed in numerical studies of the $P(q)$ where a secondary peak in that distribution function has been observed already for small sizes for certain disorder realizations [15–17].

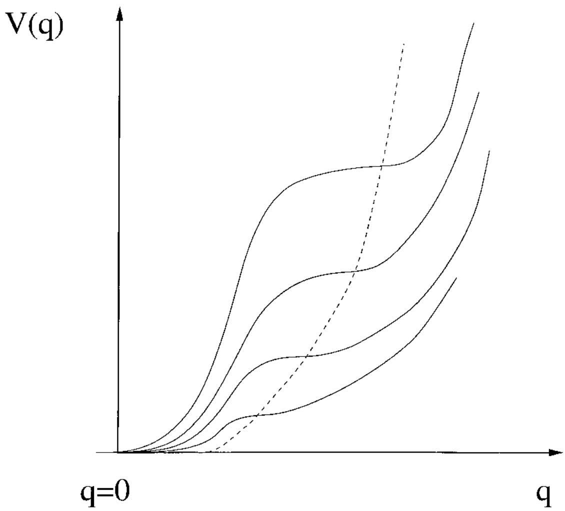

Fig. 4. Potential function for the short-range p-spin spin glass at $\varepsilon = 0$ above T_c as a function of temperature. From high temperatures (above) to low temperatures (below). The secondary minimum at $q \neq 0$ is a spinodal point. The height of that secondary saddle point is the complexity (the logarithm of the number of metastable states per site) which vanishes at T_c. The potential at $T = T_c$ becomes flat and $q_{\rm EA}$ vanishes at T_c (following the dashed line).

In summary, we have studied a short-range spin-glass model which in the mean-field approximation is well consistent with the Adam–Gibbs–DiMarzio theory and with the ideal mode-coupling theory. In the ε–T plane we have found evidence for a line of critical points. Our study has been done in the high-temperature phase where thermalization is easier to achieve (but still, huge thermalization times are needed for large sizes) compared to the low-temperature region. Our results cannot exclude the possibility that we are observing a crossover behavior where the maximum value of g would eventually vanish for $L \to \infty$ [25].[3] Although we cannot exclude that possibility its sole presence is reminiscent of the first-order character of this critical line in the mean-field approximation which induces a behavior much different to that found in the finite dimensional Edwards–Anderson model. Our results have two immediate consequences: (1) The difficulty to discern a true critical behavior form a crossover behavior makes very hard to numerically establish the existence of a critical line (first order or continuous) in the ε–T plane for low values of ε using equilibrium methods which are known to reasonably work for $\varepsilon = 0$. This conclusion applies to both spin glasses and structural glasses. (2) If the line observed where only a crossover behavior this adds evidence to the fact. A Kauzmann transition may well exist only in mean-field models where an unambiguous definition of an equilibrium configurational entropy is possible. Further studies should extend the present analysis to study the potential energy landscape and a numerical estimate of the dynamical configurational entropy for

[3] Strong finite-size effects (but in a very different context, i.e., at $\varepsilon = 0$) have been observed in the disordered hierarchical lattice.

this model (such as that which has been done for glass-forming liquids [26,27]) as well as the role of the Griffiths singularities in the dynamics.

Acknowledgements

We thank G. Parisi for discussions and F.G. Padilla for a careful reading of the manuscript. We are grateful to M. Mézard for communicating us his results. This work has been supported by the Ministerio de Educación y Ciencia in Spain through the Project PB97-0971. M.C. thanks Fondazione Angelo Della Riccia for financial support.

References

[1] J.H. Gibbs, E.A. Di Marzio, J. Chem. Phys. 28 (1958) 373.
[2] G. Adams, J.H. Gibbs, J. Chem. Phys. 43 (1965) 139.
[3] C.A. Angell, Science 267 (1995) 1924.
[4] W. Gotze, in: J.P. Hansen, D. Levesque, J. Zinn-Justin (Eds.), Liquid, Freezing and the Glass transition, Les Houches (1989), North Holland, Amsterdam.
[5] T.R. Kirkpatrick, D. Thirumalai, Phys. Rev. B 36 (1987) 5388.
[6] T.R. Kirkpatrick, P.G. Wolyness, Phys. Rev. B 36 (1987) 8552.
[7] S. Franz, G. Parisi, Phys. Rev. Lett. 79 (1997) 2486.
[8] S. Franz, G. Parisi, Physica A 261 (1998) 317.
[9] M. Cardenas, S. Franz, G. Parisi, J. Phys. A 31 (1998) L163.
[10] M. Cardenas, S. Franz, G. Parisi, J. Chem. Phys. 110 (1999) 1726.
[11] M. Mézard, cond-mat 9812024.
[12] M. Mézard, G. Parisi, M.A. Virasoro, Spin Glass Theory and Beyond, World Scientific, Singapore, 1987.
[13] K. Binder, A.P. Young, Rev. Mod. Phys. 58 (1986) 801.
[14] K.H. Fischer, J.A. Hertz, Spin Glasses, Cambridge University Press, Cambridge, 1991.
[15] M. Campellone, B. Coluzzi, G. Parisi, Phys. Rev. B 58 (1998) 12 081.
[16] M. Campellone, G. Parisi, P. Ranieri, Phys. Rev. B 59 (1036).
[17] S. Franz, G. Parisi, Critical properties of a three dimensional p-spin model, preprint, cond-mat 9805088.
[18] E. Marinari, C. Naitza, G. Parisi, M. Picco, F. Ritort, F. Zuliani, Phys. Rev. Lett. 81 (1998) 1698.
[19] G. Parisi, M. Picco, F. Ritort, Phys. Rev. E 60 (1999) 58.
[20] S. Caracciolo, M. Palassini, Phys. Rev. Lett. 82 (1999) 5128.
[21] D. Alvarez, S. Franz, F. Ritort, Phys. Rev. B 54 (1996) 9756 and references therein.
[22] E. Marinari, G. Parisi, J.J. Ruiz-Lorenzo, in: A.P. Young (Ed.), Spin Glasses and Random Fields, World Scientific, Singapore, 1998.
[23] B. Derrida, Phys. Rev. Lett. 45 (1980) 79.
[24] S. Franz, G. Parisi, J. Phys. I 5 (1995) 1401.
[25] M.A. Moore, H. Bokil, B. Drossel, Phys. Rev. Lett. 81 (1998) 4252.
[26] F. Sciortino, W. Kob, P. Tartaglia, Phys. Rev. Lett. 83 (1999) 3214.
[27] A. Crisanti, F. Ritort, Europhys. Lett. 51 (2000) 147.