A general method to determine replica symmetry breaking transitions

E. Marinari, C. Naitza, F. Zuliani
Dipartimento di Fisica and INFN, Universita di Cagliari
Via Ospedale 72, 07100 Cagliari (Italy)
E-Mail: marinari@ca.infn.it, naitza@ca.infn.it, zuliani@ca.infn.it

G. Parisi
Dipartimento di Fisica and INFN, Universita di Roma La Sapienza
P. A. Moro 2, 00185 Roma (Italy)
E-Mail: giorgio.parisi@roma1.infn.it

M. Picco
LPHT
Université Pierre et Marie Curie, PARIS VI
Université Denis Diderot, PARIS VII
Boîte 126, Tour 16, 1ère étage, 4 place Jussieu
F-75252 Paris CEDEX 05, FRANCE
E-Mail: picco@lpthe.jussieu.fr

F. Ritort
Departament de Física Fonamental, Facultat de Física
Universitat de Barcelona, Diagonal 647
08028 Barcelona (Spain).
E-Mail: ritort@ffn.ub.es
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We introduce a new parameter to investigate replica symmetry breaking transitions using finite-size scaling methods. Based on exact equalities initially derived by F. Guerra this parameter is a direct check of the self-averaging character of the spin-glass order parameter. This new parameter can be used to study models with time reversal symmetry but its greatest interest concerns models where this symmetry is absent. We apply the method to long-range and short-range Ising spin glasses with and without magnetic field as well as short-range multispin interaction spin glasses.

The subject of replica symmetry breaking has become an important issue in statistical physics [1]. Since replica symmetry breaking was proposed long time ago [2] there have been several new developments concerning spin glasses as well as their applications in other areas of statistical physics. The implications of the result whether replica symmetry breaking takes place in real physical systems can be of the utmost importance. Leaving aside the question whether and how this transition could be observed in real experiments, it is certainly relevant to establish the validity of mean-field theory for spin glasses when applied to short-range systems. In this context, quite recently a new controversy has appeared on the problem whether self-averagingness (i.e. the independence of the order parameter on the microscopic realization of the quenched disorder) is automatically satisfied in short-range systems. While the answer to this question (according to heuristic arguments by Newman and Stein [3]) appears to be closely related to the proper definition of the order parameter and how the thermodynamic limit is taken, there are few doubts that non self-averaging is the crucial signature for a spin-glass scenario where replica symmetry breaks.

The purpose of this letter is to unambiguously show that indeed replica symmetry (hereafter, referred to as RS) breaks in short-range spin-glasses and that the genuine feature of the broken phase relies on the non-self averaging character of the order parameter. While the major part of work in spin glasses has been focused in models where there is a time reversal symmetry in the Hamiltonian this is not an essential requirement for the existence of a replica symmetry breaking (RSB) transition. In models with time-reversal symmetry (hereafter referred as TRS), RS and TRS break simultaneously at the spin-glass transition temperature. Because both RS and TRS break precisely at the same temperature, it is very difficult to distinguish the different features related to both transitions. Indeed, the main distinction between the droplet [4] and the mean-field approaches relies on which symmetries break at the spin-glass transition temperature. While in the first approach only TRS breaks at the transition temperature, in the second approach both symmetries break. The most widely used parameter to locate spin-glass transitions (the Binder parameter) signals the breaking of time reversal symmetry rather than the other. Consequently, the major part of numerical calculations using the Binder parameter do not show that RS breaks at the spin-glass transition temperature but
rather whether TRS breaks. Then, it is essential to look for signatures of replica symmetry breaking in models where time reversal symmetries are lacking.

A large class of models where TRS is not present are spin glasses in an external magnetic field or multispin p-interactions spin-glass models (p-SG) with p odd. The first class of models can be described by Hamiltonians of the type,

$$\mathcal{H} = \mathcal{H}_0 - h \sum_i \sigma_i = -\sum_{(i,j)} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i$$ \hspace{1cm} (1)

where the term $h \sum_i \sigma_i$ breaks the TRS ($\sigma \to -\sigma$) of the Hamiltonian $\mathcal{H}_0$. On the other hand, models of p-SG take the general form,

$$\mathcal{H} = - \sum_{(i_1,i_2,\ldots,i_p)} J_{i_1i_2\ldots i_p} \sigma_{i_1} \sigma_{i_2} \ldots \sigma_{i_p}$$ \hspace{1cm} (2)

For $p$ odd TRS is absent. The interest of this last family of models (contrarily to (1)) relies on the fact that there is no parameter which appropriately tuned restores TRS (this happens in the family of models of eq.(1) where TRS is recovered if $h = 0$).

When studying phase transitions in ordered systems one generally computes the temperature dependence of cumulants of the order parameter distribution such as susceptibilities (for instance, second moments) which usually display power law divergences. Also, one can consider adimensional parameters such as the kurtosis (usually known as Binder parameter) or the skewness of the order parameter distribution. These adimensional parameters are related to the amplitudes of the scaling quantities in the renormalization group flows and they are good indicators for the transition. They find their most successful application in finite-size scaling studies.

The usefulness of these quantities to distinguish RSB transitions is hampered by the fact that finite-size corrections to the leading scaling behavior of the Binder parameter can be big. For RSB transitions it is then convenient to consider adimensional quantities which depend on other genuine features of the transition (and not only on TRS) such as self-averageness. Our purpose here is to define a suitable parameter which is the analogous of the Binder parameter for transitions where TRS breaks and which can be used to locate spin-glass transitions where RS breaks. In spin-glasses the order parameter is not the global magnetization but a measure of the freezing of the RS breaks. In spin-glasses the order parameter distribution is a parameter which is the analogous of the Binder parameter distribution where the usual Boltzmann-Gibbs average for a given sample. It has been recently shown by F. Guerra that sample to sample fluctuations of the cumulants of the order parameter distribution $P_{BL}(q)$ are Gaussian distributed in the thermodynamic limit. For instance, the following relationship is fulfilled in spin glasses in the low temperature phase below $T_c$,

$$G = \frac{\chi_{SG}^2 - \chi_{BG}^2}{V^2 (q - \langle q \rangle BG)^4 BG - \chi_{SG}^2} = \frac{1}{3}$$ \hspace{1cm} (3)

where $\langle \rangle$ means average over the quenched disorder and $\chi_{SG}$ (the spin-glass susceptibility) is defined as

$$\chi_{SG} = V(q^2 BG - \langle q \rangle^2 BG)$$ \hspace{1cm} (4)

The interest of defining the parameter $G$ is that it vanishes above the transition temperature in the disordered phase where sample to sample fluctuations of $P_{G}(q)$ disappear in the $V \to \infty$ limit. Similar information to that obtained from (3) can be also gathered from the sample to sample fluctuations of $\chi_{SG}$:

$$\alpha = \frac{\chi_{SG}^2 - \chi_{BG}^2}{\chi_{SG}}$$ \hspace{1cm} (5)

which only involves the first and second moments of the order parameter. As we will see later (6) yields also non trivial behavior in the low temperature phase even though (in contrast to $G$) it does not necessarily converge (in the thermodynamic limit) to a temperature independent value. Consequently, $G$ is a parameter which plays the same role as the usual Binder parameter $g$ in ferromagnets and is given (in the $V \to \infty$ limit) by $G(T) = (1/3)(1 - \Theta_H(T - T_c))$ where $\Theta_H$ is the Heaviside theta function. In RSB transitions (3) goes to zero (as the size $V$ increases) as $1/V$ for $T > T_c$ but converges to a finite value for $T < T_c$. We expect the critical temperature (where RS breaks) to be signaled by the crossing of the different curves corresponding to different lattice sizes. Furthermore, close to $T_c$, it is reasonable to expect, $G(T) \sim G(L/\xi)$ where $\xi$ is a correlation length. We stress that the calculation of $G$ is specially useful in models where TRS is absent. In the presence of TRS the usual Binder parameter $g$ can be used to locate the phase transition with much less numerical effort. But the interest of $G$ is that it emphasizes the non-selfaveraging character of the low temperature phase.

To check these predictions we have performed numerical simulation of models of the previous type (1) (with and without magnetic field) and the p-spin model (2). All the simulations use the parallel tempering method, an efficient algorithm to thermalize small samples (7). We have studied three different models, the mean-field Sherrington-Kirkpatrick (SK) model (3), the four dimensional (4D) Ising spin glass, and the model eq.(3) in four dimensions with $p = 3$. In this last case, the Hamiltonian
is short-ranged, there are two spins per site in a 4D simple cubic lattice and the Hamiltonian couples all possible triplets of spins occupying nearest-neighbor sites of the lattice. More precisely the Hamiltonian reads,

$$\mathcal{H} = -\sum_{i=1}^{V} \sum_{\mu=1}^{D} (J^{i;\mu}_{(12,1)} \sigma^i_1 \sigma^j_2 \sigma^{i+j}_1 + J^{i;\mu}_{(2;1)} \sigma^i_2 \sigma^j_2 \sigma^{i+j}_2 + J^{i;\mu}_{(1;2)} \sigma^i_1 \sigma^j_2 \sigma^{i+j}_1)$$

(6)

where the pair $(i, \mu)$ denotes the link of the lattice and the spins $(\sigma^i_1, \sigma^j_2)$ occupy the same site $i$ in the lattice.

FIG. 1. $G$ in the 4D Ising spin glass without a field. The horizontal line indicates the expected low $T$ result $G = 1/3$ while the vertical line indicates the expected transition temperature derived form other methods [1][2]. Error bars are shown for $L = 4, 10$.

First, we show the results in the four dimensional Ising spin glass without a magnetic field ($h=0$). This is a check of our method since the transition is well known using standard methods [7]. The model is described by eq. (1) with $J_{ij} = \pm1$ connecting nearest-neighbor sites of in a cubic lattice of side $L$ with periodic boundary conditions. The simulations were done for sizes $L = 4, 5, 8, 10$ (2944, 1920, 1376, 320 samples respectively) with 100000 Monte Carlo steps (MCS) of thermalization time and the same amount of steps to collect statistics (for $L = 10$ we did runs up to 35 million of MCS). Figure 1 shows the results for $G$. Note the existence of a critical temperature above which $G$ goes to zero and below which it converges to $1/3$. The different curves cross at a temperature in agreement with that derived from the analysis of the usual Binder parameter [4] and also series expansions [9] ($T_c \approx 2.03$). We have also analyzed the parameter $\alpha$ of eq. (3) which shows that $\alpha(L) \sim 1/V$ for $T > T_c$ while $\alpha(L) \approx \alpha(\infty) + A/L^\lambda$ with $A > 0$ for $T < T_c$, giving qualitatively the same information as $G$.

Next we consider models without TRS. We first consider the study of the SK model in a magnetic field. The SK model [8] corresponds to eq. (1) with $J_{ij}$ long-ranged and Gaussian distributed with $J_{ij} = 0, \bar{J}_{ij} = 1/V$. The existence of a transition in a field is well established in mean-field theory but there are few results which corroborate its existence using numerical simulations [11]. Figure 2 shows $G(T)$ for $V = 32, 256, 512, 1024$ with 1000, 1000, 400, 150 samples respectively. While it is very difficult to see evidence for this transition with the usual cumulants (skewness or Binder parameter) the situation turns out to be more clear with the parameter $G$ where a merging close to $T \approx 6 - .7$ (below $T_c(h = 0) = 1$) is observed. The figure clearly shows the existence of two temperature regions. A high temperature region where $G$ goes to zero with the volume (as $1/V$) and a low temperature one where $G$ converges to $1/3$ (within the precision of the statistics). This shows the existence of the Almeida-Thouless line in the SK model, a result well known in the mean-field theory of spin glasses but difficult to observe numerically.

FIG. 2. $G$ in the SK model at $h = 0.3$. Error bars are shown for $V = 32, 1024$. The different curves merge at a temperature well compatible with the theoretical result $T_c(h = 0.3) = 0.65$ [12].

The results in the four dimensional Ising spin-glass model in a field are shown in figure 3. Simulations were done at a magnetic field $h = 0.4$ with statistics ranging from 20000 MCS for $L = 3$ up to 450000 for $L = 9$. We observe also here a behavior very similar to that found in figure 2. The existence of the two regions (a high temperature one where $G$ goes to zero and a low temperature
one where $G$ converges to a finite value close to $1/3$) is also clear from the plot.

Figures 2 and 3 show quite unambiguously that there are two regions where self-averaging properties are quite different. This is a strong indication in favor of the existence of a RSB phase transition in spin glasses in a magnetic field. But a scale invariant crossing point is not so clearly observed in figures 2 and 3 compared to what is observed in figure 1 for zero magnetic field and figure 4 (see below). There are two factors which make numerical simulations of spin glasses in a magnetic field much more difficult. The first one is related to the difficulty of thermalizing spin-glasses at low temperatures. When the field is switched on the critical temperature is pushed down (as figures 2 and 3 clearly show). This makes thermalization in the low temperature region more difficult. The second factor is related to the fact that Eq.(1) represents the TRS at zero magnetic field. Consequently, it stores the TRS at zero magnetic field. Consequently, it is natural to expect the existence of a crossover length $L_c$ (which increases as the magnetic field decreases) such that above $L_c$ the finite-field fixed point dominates the scaling behavior while below $L_c$ the scaling behavior is dominated by the zero field fixed point. In the case of figure 3 the crossover length was previously estimated ($L_c \approx 5$). This crossover effect manifests as a displacement of the crossing point to lower temperatures as the size increases. For large sizes (and always within errors) the crossing point stays around $T_c \approx 1.2$, a value for the critical temperature which has been estimated also through other methods.

Assuming that the value of the parameter $G$ at the crossing point corresponds to a universal amplitude we find (after examination of the data for the SK and the 4D Ising spin glass at zero and finite field), that $G_c = G(T = T_c)$ clearly increases with the field. This result suggests (in case the previous assumption is correct) that the transition without a field and in a field are determined by different fixed points.

To check that the parameter $G$ is indeed a good tool to determine RSB transitions it would be more convenient to consider a model where there is no external small parameter (like the field) which can restore the TRS. For such a model there will not be a crossover length $L_c$ and a crossing point for the parameter $G$ should be easier to see already for small sizes. To confirm these expectations we have investigated model (6) with $J^{i,J} = \pm 1$ in four dimensions in lattices of sizes $L = 3, 4, 5, 6$ with $100000$ MCS of statistics per temperature. The results are shown in figure 4. From it it is clear that there is no global symmetry in this model and the only possible phase transition we can expect is a first-order one. We have verified that there is no latent heat and that the order parameter $(q)_{BG}$ does not experience any discontinuous jump at any finite temperature. Having discarded the usual thermodynamic first-order transition scenario the only possibility left is the existence of a RSB transition where the spin-glass susceptibility diverges. Indeed our results show an algebraic divergence of the spin-glass susceptibility $\chi_{SG}$ and a least-squares fit gives $\chi_{SG} \sim (T - T_c)^{-\gamma}$ with $T_c \approx 2.63$ and $\gamma \approx 1.0$. This value of $T_c$ is in striking agreement with the crossing point observed in figure 4.

If one assumes, as said before, that $G(T) \sim \tilde{G}(L/\xi)$ with

![Figure 3](image-url)  
**FIG. 3.** $G$ in the 4D $\pm J$ Ising spin glass at $h=0.4$. The number of samples is $2560, 1280, 704, 64$ for $L = 3, 5, 7, 9$ respectively. Error bars are shown for $L = 3, 9$.

![Figure 4](image-url)  
**FIG. 4.** $G$ in the model without TRS symmetry with three-spins interaction and two spins per site. We find that $T_c \approx 2.62$. Error bars are shown for $L = 3, 6$. 

The second factor is related to the fact that Eq.(1) restores the TRS at zero magnetic field. Consequently, it is natural to expect the existence of a crossover length $L_c$ (which increases as the magnetic field decreases) such that above $L_c$ the finite-field fixed point dominates the scaling behavior while below $L_c$ the scaling behavior is dominated by the zero field fixed point. In the case of figure 3 the crossover length was previously estimated ($L_c \approx 5$). This crossover effect manifests as a displacement of the crossing point to lower temperatures as the size increases. For large sizes (and always within errors) the crossing point stays around $T_c \approx 1.2$, a value for the critical temperature which has been estimated also through other methods.

Assuming that the value of the parameter $G$ at the crossing point corresponds to a universal amplitude we find (after examination of the data for the SK and the 4D Ising spin glass at zero and finite field), that $G_c = G(T = T_c)$ clearly increases with the field. This result suggests (in case the previous assumption is correct) that the transition without a field and in a field are determined by different fixed points.
$\xi \sim (T - T_c)^{-\nu}$ then $(dG/dT)_{T = T_c} \sim L^\Delta$. A power law fit yields $\nu \simeq 1/2$ suggesting that both $\gamma$ and $\nu$ are close to mean-field values. Let us note that the same conclusions are obtained by studying the parameter $\alpha$ in eq. (5).

Summarizing, we have proposed a new parameter $G$ based on exact inequalities initially derived by Guerra [5]. This parameter is suited to numerically study replica symmetry breaking transitions. The physical meaning of $G$ is related to the very nature of the replica symmetry broken phase, i.e. the absence of self-averaging in the order parameter. When replica symmetry is not broken the spin-glass order parameter is self-averaging but this property is lost in the broken phase. The parameter $G$ in eq. (4) has the good properties of being bounded and positive (a property which does not have the usual Binder parameter used for spin-glasses without TRS) and can be used as a good indicator for RSB transitions using finite-size scaling methods. At high temperatures $G$ goes to zero as $1/V$ where $V$ is the volume of the system while at low temperatures it converges to $1/3$ in the $L \to \infty$ limit. The method can be also used to investigate transitions where TRS breaks. In particular, we have investigated the 4D Ising spin-glass at zero field and found that indeed RS breaks at $T_c$. This result unambiguously shows that both TRS and RS break at $T_c$. But its greatest potential applicability concerns disordered models without TRS. In particular, we have considered spin glasses in a magnetic field (the SK model as well as the 4D Ising spin glass) which clearly show the existence of two different regimes corresponding to different self-averaging properties of the order parameter. But the nicest application of the method is for models where there is no tunable parameter which restores time reversal symmetry (like the magnetic field). By introducing a new short-range $p$-spin model (eq. (3)) we have shown that $G$ is indeed a good indicator for RSB. We have considered a model with $p = 3$ in 4D and we have shown that there is no thermodynamic first phase order transition. In this case $G$ displays a crossing point where the spin-glass susceptibility diverges. Finally, we want to stress that the information gathered from $G$ in models without TRS cannot be extracted in an easy way from the usual standard cumulants of the sample averaged $P(q)$. The genuine property of replica symmetry breaking transitions in disordered systems is the non self-averaging character of the spin-glass order parameter, a feature which is specifically taken into account within the present method. A more deep understanding of the appropriate renormalization group approach in spin glasses is certainly needed to clarify the appropriate theoretical framework to deal with this type of phase transitions.

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