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Three-dimensional Ising spin-glasses and mean-field theory

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Résumé. — Nous présentons les résultats d'une simulation numérique de verres de spin d'Ising tridimensionnels à courte portée et nous comparons les résultats aux prédictions de la théorie du champ moyen. Nous trouvons que le paramètre d'ordre $P(q)$ du modèle avec des interactions à courte portée a un comportement similaire à celui du modèle avec des interactions à portée infinie.

Abstract. — The results of a simulation of a three-dimensional nearest neighbour Ising spin-glass are presented and compared with mean-field theory predictions. It is found that the order parameter $P(q)$ has a similar behaviour in the short-range coupling and in the infinite-range coupling model.

In this Letter we report on numerical simulations of three-dimensional, nearest-neighbour Ising spin-glasses. A great amount of numerical simulations have been devoted to this problem [1] and proven to be a very useful tool in the study of spin-glasses. It has been shown that there exists a temperature T_g such that for $T < T_g$ the system « freezes ». Whether (for three-dimensional systems) T_g corresponds to a sharp phase transition is a very difficult and still hotly debated question, which will not be examined in the present paper.

On the other hand our understanding of the mean-field theory of spin-glasses [2] (i.e. the infinite-range model) has greatly improved recently. In particular it has been shown [3, 4] that the order parameter is not self-averaging (i.e. it depends on the particular coupling configuration) even in the thermodynamic limit. It has also been shown that the space of pure spin-glass states has an ultrametric topology [3]. The above properties have been obtained in the framework of Parisi's replica symmetry breaking scheme [5].

Our aim is to find whether mean-field theory provides a good description of spin-glasses at low temperature. The characteristic property of the spin-glass phase is (at least in the mean-field approximation) the existence of a large number of equilibrium states which are not simply

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related by any symmetry. It could be that these states are metastable in 3 dimensions. This question is not examined in the present paper.

Parisi [6] has introduced the notion of overlap $q_{\alpha\beta}$ between two pure states α and β

$$q_{\alpha\beta} = \frac{1}{N} \sum_i m_i^\alpha m_i^\beta \quad (1)$$

(where N is the total number of spins and m_i^α the magnetization at site i in the pure state α) and the probability $P(q)$ for $q_{\alpha\beta}$ to get the value q . $P(q)$ is the order parameter for the spin-glasses. A broad $P(q)$ indicates the existence of many states in the system.

Parisi showed how $P(q)$ can be computed by considering two identical systems and proposed $P(q)$ as the order parameter for spin-glasses. We have computed the function $P(q)$ and looked at the ultrametricity property of the states. We examined only a few J_{ij} coupling configurations but we tried to get high accuracy for those configurations. As we are dealing with finite systems we have a finite transition probability from one state to another and we cannot increase the accuracy within each state by waiting very long. An alternative way to increase the accuracy has been suggested by Parisi [7] : one can integrate analytically the degrees of freedom of a small subsystem and use the usual M.-C. algorithm only to generate the boundary conditions for the different subsystems. In the present computation, we have integrated analytically a subsystem made from seven spins (one spin plus its six neighbours). This trick only affects the « measuring process ». The updating procedure is left unchanged. It has reduced the numerical errors due to the M.-C. algorithm by a factor $4 \sim 8$ (depending on temperature, the reduction increasing with temperature).

We have considered a three-dimensional Ising model, on a N^3 cubic lattice, where $N = 12, 14, 16$, with the Hamiltonian :

$$H = - \sum_{(ij)} J_{ij} \sigma_i \sigma_j \quad (2)$$

where J_{ij} are next nearest-neighbour random couplings, taking with equal probability the values ± 1 . We have used the « heat bath » Monte-Carlo algorithm, the spins being updated at random order. We considered NS copies of the same system ($NS = 10$ for $N = 16$, $NS = 15$ for $N = 14$, $NS = 24$ for $N = 12$). The couplings J_{ij} were identical in all the copies. The copies differed only by the initial conditions which were chosen at random. The systems were slowly cooled in parallel and thermal equilibrium was assumed after 1500-3000 M.-C. steps per spin (depending on temperature). We then started doing « measurements » of all the possible $\frac{1}{2} NS (NS - 1)$ overlaps.

Successive measurements were separated by $S(N)$ M.-C. steps per spin ($S(16)=42$, $S(14)=30$, $S(12) = 18$). Typical number of measurements is 2 500 for $N = 16$ and 2 000 for $N = 14$. $P(q)$ was defined as the histogram of the $q_{\alpha\beta}$. At the same time the histogram of $(q_{\alpha\beta}, q_{\beta\gamma}, q_{\alpha\gamma})$ for the $\frac{1}{6} NS(NS - 1) (NS - 2)$ triplets was made in order to study the ultrametricity property

(see below). We also measured the distribution of the local « molecular forces » $F_i = \sum_j J_{ij} \sigma_j$. The advantage of treating several systems in parallel is two-fold : a) it increases the statistics for the overlaps $\left(\sim \frac{1}{2} NS^2 \right)$ and the triangles $\left(\sim \frac{1}{6} NS^3 \right)$; b) the space of states is more evenly filled in a more reasonable M.-C. time.

Figure 1 shows $P(q)$ for $\beta = 0.35$ and $\beta = 0.4$ for one particular configuration of the couplings on a $(14)^3$ lattice. Figure 2 shows $P(q)$ for $\beta = 0.7$ on $(16)^3$, $(14)^3$ and $(12)^3$ lattices. Figure 3 displays $P(q)$ at the same temperature ($\beta = 0.7$) for a $(14)^3$ lattice but for three different configurations of the couplings. Each point of the flat region of the histogram represents 85 000 events.

Fig. 1. — Plot of $P(q)$ for $\beta = 0.35$ (crosses) and $\beta = 0.4$ (circles).

Fig. 2. — Plot of $P(q)$ for $\beta = 0.7$ for $N = 12$ ($\times$), $N = 14$ ($\bullet$) and $N = 16$ ($+$).

Fig. 3. — Plot of $P(q)$ for $\beta = 0.7$, $N = 14$ for different J_{ij} coupling configurations.

The smallness of our errors is confirmed by the fact that the points of the histogram nicely align on a smooth curve. In order to verify that our systems have reached equilibrium and that our curves for $P(q)$ are meaningful, we have done two successive histograms, each one representing 500 « mesures » on a $(12)^3$ lattice. The result is shown in figure 4. Although the exact numerical values are slightly different, the shape of the curves is essentially the same. Table I gives the distribution of the molecular fields at different temperatures. (It can be shown in the mean-field theory that the F_i distribution is self-averaging [8]. We have verified that this is also true in the three-dimensional short-range model). We have also measured $P(q)$ for $\beta = 0.3, 0.5, 0.6$ and $\beta = 0.8$. Below $\beta_g \sim 0.45$, $P(q)$ is a sharp « δ -function », which means that our system has a single state. For $\beta > \beta_g$, $P(q)$ becomes wider, as in the mean-field description of the spin-glass phase. Looking now at table I we see that for $\beta < 0.4$ the distribution of the F_i 's is peaked at $F = 0$, while for $\beta > 0.4$ the individual spins are, with high probability, frozen (for example for $\beta = 0.7$ and $F = 2$, the probability of flipping a spin is $\frac{e^{-2\beta}}{e^{2\beta} + e^{-2\beta}} = 0.057$).

Fig. 4. — Two measurements of $P(q)$ for $\beta = 0.7$, $N = 12$ made one after the other. Although each one represents only 500 measurements there is no significant time dependence in the shape of $P(q)$.

Table I. — *Distribution of the « molecular fields » F at various temperatures.*

$\beta \backslash F$	- 6	- 4	- 2	0	2	4	6
0.35	0.045	0.140	0.205	0.217	0.205	0.141	0.045
0.4	0.053	0.150	0.197	0.197	0.197	0.150	0.053
0.5	0.069	0.168	0.182	0.160	0.182	0.168	0.069
0.7	0.088	0.191	0.163	0.111	0.163	0.193	0.089
0.8	0.093	0.202	0.157	0.093	0.155	0.199	0.1

The two methods to determine the freezing temperature β_g , although numerically independent, and not very accurate, give consistent results. So, as far as the order parameter is concerned, there is not any difference between the low temperature infinite range, or the three-dimensional short-range model, at least far below T_g and for times up to 100 000 M.-C. steps per spin.

A few remarks are in order : a) $P(q)$ looks quite different from what one gets in the infinite range calculations (in that model $P(q)$ has been obtained through the PaT hypothesis [9] and has also been measured numerically [10]). There is a dip around $q = 0$ and, as the volume increases, there is an indication that $P(q)$ tends to sharpen, but it remains much more rounded (at least for sizes up to $(16)^3$) than in the Sherrington-Kirkpatrick model. In particular there is no sign of a δ -function at $q = q_{\max}$. The sharpness of $P(q)$ is explained in mean-field theory by the dominance of very few states. Most of the states have a very small weight. Our calculations indicate that for short-range forces the weights are more evenly distributed among the states ; b) we have not exactly determined the transition temperature (our estimate, although not very precise, is compatible with the previous estimates), nor whether the transition is sharp (appearance of states becoming stable in the thermodynamic limit, corresponding to a true phase transition) or rounded (appearance of metastable states with large but finite lifetime, even in the thermodynamic limit).

Finally we looked at the ultrametricity property. It was found in [3] that the probability $\tilde{P}(q_1, q_2, q_3)$ for the three overlaps $q_{\alpha\beta}, q_{\beta\gamma}, q_{\alpha\gamma}$ of any three pure states α, β, γ , to take the value q_1, q_2, q_3 (we suppose $q_1 \leq q_2 \leq q_3$ is proportional to $\delta(q_1 - q_2)$). It was also found that the self overlap q_{EA} is self-averaging [3] and state independent [8]. We assumed that the same is true for the short-range model. (We have numerically verified that these properties are true in the short-range model for the internal energy and the magnetization as predicted by the mean-field theory). Then, instead of the overlaps, one can consider the distances defined as follows : $x_1 = \sqrt{q_{EA} - q_1}, x_2 = \sqrt{q_{EA} - q_2}, x_3 = \sqrt{q_{EA} - q_3}$ ($x_1 \geq x_2 \geq x_3$) and the corresponding probability $P(x_1, x_2, x_3)$. We have considered all possible $(1/6) NS(NS - 1)(NS - 2)$ triplets of copies of our spin-glass system and made a histogram of x_1, x_2, x_3 . Ultrametricity would mean that this histogram is very peaked (a δ -function) around $x_1 = x_2$. It is clear that for a given x_3 the difference $x_1 - x_2$ cannot be arbitrarily large, because one of the triangle inequalities stipulates that $x_3 \geq x_1 - x_2$. (It is easy to see that this is the only constraint from the triangle inequalities when $x_1 \geq x_2 \geq x_3$). So the triangle inequalities enforce some « ultrametricity » and we would like to take this into account in our presentation. This is the reason why we chose to work with the distances x_i , rather than directly with the overlaps q_i .

We found convenient to reduce the numbers of variables by rescaling the x_i 's in order to have $x_1 + x_2 + x_3 = 3$. Then any (x_1, x_2, x_3) can be represented as a point inside an equilateral triangle, the distances from the three sides being x_1, x_2, x_3 , respectively. The distance between this point and the $x_1 - x_2 = 0$ line is $(x_1 - x_2)/\sqrt{3}$. The allowed region, once the inequalities $x_1 \geq x_2 \geq x_3$ and $x_3 \geq x_1 - x_2$ are taken into account, is the small shaded triangle shown in figure 5.

Fig. 5. — The small shadowed triangle is the allowed region for (x_1, x_2, x_3) due to the triangle inequalities.

The histogram representing the distribution of our measurements on this triangle is shown figure 6. If this presentation of the data takes easily into account the constraints from the triangle inequalities, it has the disadvantage of depending on the value of q_{EA} . q_{EA} was taken equal to the maximum value of q for which $P(q)$ is not negligible but there is an uncertainty in this determination. Increasing q_{EA} makes the histogram look more « ultrametric » (more peaked around the line $x_1 = x_2$). Decreasing q_{EA} too much leads to an apparent violation of the triangle inequalities (points falling outside the allowed region). In order to show the effect of this uncertainty we have made several histograms of the same data with different values of q_{EA} . We found that $q_{EA} = 0.37$ was the smallest value of q_{EA} for which no significant violation of the triangle inequalities was found. Figure 6a presents a histogram with $q_{EA} = 0.33$. Figure 6b presents a histogram of the *same data* but now with $q_{EA} = 0.37$. The normalization being arbitrary, only ratios of the numbers in figure 6 are meaningful. We see that our measurements are indeed peaked around the $x_1 - x_2 = 0$ line and there is an indication of ultrametricity, but again our results are more rounded than in the mean-field theory case. One should study the volume dependence of these results.

We may conclude that mean-field theory predictions are qualitatively verified in short-range three-dimensional spin-glasses. Further simulations with larger lattices, as well as a study of the dependence on the J_{ij} distribution are required for more quantitative comparison.

Fig. 6. — Two-dimensional histograms for the triangle (see text). Dashed lines represent the triangle inequalities constraint. The same data are plotted in Figs. 6a and 6b, only the choice of q_{EA} is different : $q_{EA} = 0.33$ in Fig. 6a and $q_{EA} = 0.37$ in Fig. 6b.

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