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Mean field theory for Heisenberg spin glasses

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Résumé. — Le modèle de verres de spin à portée infinie est étudié dans le cas général de spins à m composantes. Des résultats sur les lois d'aimantation, la forme du diagramme de phases, la nature des transitions sont présentés.

Abstract. — The infinite-ranged spin glass model is studied in the general case of m-component spins. Results for the magnetization laws, the shape of the phase diagram, the nature of the transitions are presented.

The infinite-ranged model [1], introduced by D. Sherrington and S. Kirkpatrick (SK), appears presently as the best definition of what mean field theory means for spin glasses. Much effort has been devoted to the simplest case of one-component (Ising) spins for which the qualitative features of the phase diagram and of the spin glass phase seem to be fairly under control [2]. Besides, the spherical approximation, in zero-field [3] and also in finite field [4], has been found to be solvable. However, few results have been presented so far for the general case of m-component (Heisenberg) spins, whereas most experimental materials correspond to the case $m = 3$. Those results [5], bearing only on the zero-field situation, prove : i) that replica-symmetry breaking occurs below the spin glass transition temperature, ii) that the spherical model is recovered in the limit $m \to \infty$.

In our study of the infinite-ranged model for Heisenberg spin glasses, we have been motivated by a desire to make closer contact with experiments, and also by a suspicion that more features might emerge for general m than a mere interpolation (between the limits $m = 1$ and $m \to \infty$) would tell. Well founded was this suspicion, as the following shows.

1. **Presentation of the problem.** — The SK Hamiltonian includes exchange forces and an applied magnetic field :

$$\mathcal{H} = - \sum_{(ij)} J_{ij} \sum_{\mu} S_{i\mu} S_{j\mu} - H \sum_{i} S_{i1} , \qquad (1)$$

where i and j are site indices ; $\mu = 1, \ldots, m$ denotes the spin components ; the magnetic field is applied in direction 1. By convention, we assume $\sum_{\mu} S_{i\mu}^2 = m$.

The exchange interactions are taken as independent random variables, with mean value J_0/N and mean deviation $J_1/\sqrt{N}$, where N is the number of spins. For notation simplicity, we take the conventions $J_1 = 1$ and $k_B = 1$, where k_B is the Boltzmann constant.

The results, presented below, have been obtained through the use of the replica strategy, which involves the computation of the nth moment of the partition function $\overline{Z^n}$ and the limit $n \to 0$ (the bar symbol means an average over the probability distributions of the interactions). The details of the derivations are too lengthy to be given in this letter.

2. **High temperature phase : fluctuations and subdominant terms.** — We assume here $J_0 = H = 0$.

The free energy, per spin, f may be written as

$$f = f_0 + \frac{f_1}{N} + 0\left(\frac{1}{N^2}\right),$$

where f_0 is the thermodynamic limit and f_1 is the subdominant term. One finds :

$$f_0 = - \frac{m}{4\,T} - T \,\mathrm{Log}\left(\frac{2\,\pi^{m/2}\, m^{m-1/2}}{\Gamma\left(\frac{m}{2}\right)}\right), \qquad (2)$$

$$f_1 = -\frac{Tm^2}{4}\operatorname{Log}\left(1 - \frac{1}{T^2}\right) + \\ + T\cdot\frac{(m-1)(m+2)}{4}\operatorname{Log}\left(1 - \frac{m}{T^2(m+2)}\right), \quad (3)$$

$$K_2 = -\frac{m^2}{2}\left[1 + T^2\operatorname{Log}\left(1 - \frac{1}{T^2}\right)\right], \quad (4)$$

where K_2 is the mean deviation of the total free energy [6].

In the limits $m \to 1$ and $m \to \infty$, formula (2) reproduces the Ising and spherical results, respectively [5]. In the Ising case, it had been early recognized that the spin glass transition corresponds to a singularity, not in the thermodynamic term f_0, but in the subdominant term f_1. Formula (3) shows that besides the singularity at $T_c = 1$, there appears, for $m \neq 1$, another singularity at a lower temperature

$$T^* = \sqrt{\frac{m}{m+2}}.$$

In the limit $m \to \infty$, these two temperatures coalesce, yielding a different singularity :

$$\frac{f_1}{m} \to \frac{T}{4}\operatorname{Log}\left(1 - \frac{1}{T^2}\right) + \frac{T}{2(T^2-1)}. \quad (5)$$

The transition occurring at $T_c = 1$ is the spin glass transition. Whether a second transition takes place at T^* or whether it is suppressed by the onset of the first instability, is a question to be discussed, as well as the nature of this second instability.

3. **Magnetization laws in the paramagnetic phase.** — All our results will now concern physical quantities, taken in the thermodynamic limit ($N \to \infty$). We have performed a systematic expansion of the free energy up to sixth order in the magnetic field. For this purpose, it is necessary to obtain an expansion (of the Ginzburg-Landau type) for the free energy as a function of three additional variables (besides H) :

$q_1 = \overline{\langle S_1 \rangle^2}$, the longitudinal Edwards-Anderson (EA) order parameter [7],

$q_T = \overline{\langle S_\mu \rangle^2}$, $\mu \neq 1$, the transversal EA order parameter,

x, a measure of the « orientation » of the spins, which is defined by :

$$\overline{\langle S_1^2 \rangle} = 1 + (m-1)\,x\,, \quad (6)$$

where the bracket symbol means a thermodynamic average.

Clearly, in the Ising case, only q_1 is to be considered [8]. It is the existence of q_T and x that make the general Heisenberg case hard. The true free energy, function of T and H, is obtained as a stationary value of the Ginzburg-Landau free energy with respect to the three variational parameters q_1, q_T, x.

The magnetization M, in the magnetic field H, is obtained as

$$M = \frac{H}{T} - a\frac{H^3}{T^3} + b\frac{H^5}{T^5} + \cdots, \quad \text{for} \quad T > 1\,, \quad (7)$$

with

$$a = \frac{1}{m+2}\left[\frac{T^2+m+1}{T^2-1} - \frac{m(m-1)}{(m+2)\,T^2 - m}\right], \quad (8)$$

the general expression for b being cumbersome, we give here only its Ising ($m = 1$) value

$$b(m=1) = \frac{2}{15(T^2-1)^3} \times \\ \times [T^6 + 12\,T^4 + 18\,T^2 - 16]\,. \quad (9)$$

The expression of a, in the Ising case, has already been published [9] and full credit should be given to the Japanese school [8, 9] for stressing the remarkable behaviour of the non-linear magnetization in Ising spin glasses.

Comparison of formula (8) with formula (3) shows that similar singularities at the temperatures T_c and T^* occur both in the subdominant term of the free energy and the non-linear coefficient of the magnetization. This fact seems to be worthy of attention. Of course, we are used to the linear response formulae which relate the fluctuations of a thermodynamic quantity (say, the magnetization) to a linear coefficient (say, the magnetic susceptibility). In these disordered systems, that spin glasses are, it is good to see the emergence of an equally simple, but new, relation.

Formula (9) shows that the higher order coefficients are also divergent. Coefficient b is useful for the analysis of experimental data, a topic to be discussed elsewhere. These divergences announce a change of the magnetization law, when T_c is reached. For $T = 1$, one gets :

$$M = H - \frac{H^2}{\sqrt{2}} + \frac{H^3(m^2 + 2\,m + 20)}{8(m+2)} + \cdots. \quad (10)$$

The limit for $m = 1$ was already known [6]. The limit for $m \to \infty$ is not trivial because the temperatures T^* and T_c coalesce, whereas the calculations have been performed assuming that $T^* < T_c$. Indeed, in formula (7), one sees that the magnetic field, in the limit $m \to \infty$, has to be normalized as $H = h\sqrt{m}$ which is reasonable since the saturated magnetization also scales as $\sqrt{m}$. However, with this normalization, formula (10) appears to blow up, but its domain of validity has actually shrunk to zero.

Formula (10) implies a break of analyticity at $H = 0$, because of the appearance of even terms. It is perhaps the neatest manifestation of the spin glass transition.

4. **Freezing of the transversal degrees of freedom.** — In the course of the calculations leading to the results presented above, the values of q_1, q_T and x, that make the free energy stationary, are computed, order by order in the magnetic field H.

For $T \geqslant 1$, it is found that q_T remains vanishing in presence of the field, whereas q_1 and x become finite.

Since for $T < 1$ and $H = 0$, it is known that $q_T = q_1 \neq 0$, this implies that in the phase diagram (H, T) there is a transition line corresponding to the onset of a non-zero q_T, i.e. the onset of a freezing of the transversal degrees of freedom. The equation of this transition line, to lowest order in H, is :

$$\tau = 1 - T = \frac{H^2}{4} \cdot \frac{(m+4)}{(m+2)} + 0(H^4). \quad (11)$$

The coefficient of the H^2 term is weakly dependent on m. But the notion of transversal degrees of freedom does not make sense for $m = 1$, and for $m \to \infty$, again, the coalescence of the singularities requires a careful examination.

We now present a few expressions, for the temperature range $T \lesssim 1$ ($\tau \ll 1$). Assuming no replica symmetry breaking, the Fischer formula for the linear (zero-field) susceptibility is generalized in the Heisenberg case to :

$$\chi_\mu = \frac{1}{T}[\overline{\langle S_\mu^2 \rangle} - \overline{\langle S_\mu \rangle^2}], \quad (12)$$

and therefore :

$$\chi_1 = \frac{1}{T}[1 - q_1 + (m-1)x], \quad (13)$$

$$\chi_T = \frac{1}{T}[1 - x - q]. \quad (14)$$

For $T^* < T < 1$, no anisotropy is expected in zero-field ($x \equiv 0$) and one obtains

$$q_1 = q_T = \tau + \frac{\tau^2}{m+2} + 0(\tau^3). \quad (15)$$

In finite field,

$$q_T \sim \tau - \frac{H^2}{4}\frac{m+4}{m+2} + \cdots \quad (16)$$

$$q_1 \sim \tau + \frac{\tau^2}{m+2} + \frac{H^2}{2\tau} + \cdots. \quad (17)$$

As a consequence, the magnetization law is

$$M \sim H\left[1 - \frac{\tau^2}{m+2}\right] - \frac{H^3}{2\tau} + \cdots, \quad (18)$$

an expression to be compared to formulae (7) and (8), which are valid for $T > 1$. The Ising limit of formula (18) was already known [2]. One important fact : this formula predicts that a maximum of the function $M(T)$, in a given field H, occurs for

$$H^2 \sim \frac{4\tau^3}{m+2} + \cdots. \quad (19)$$

Now, in the Ising case, it has been found [2] that, to this order, the transition line corresponding to replica-symmetry breaking coincides with the locus of the maximum $M(T)$. Is it still the case for Heisenberg spins ? We cannot answer this question at the moment. If we assume, as a guess, that the answer is positive, we are led to think that the replica-symmetry instability does not affect the transversal freezing transition (at least in low fields).

5. **Is there a transition around T^* ?** — The physical manifestation of such a transition would be the spontaneous onset of an anisotropy for the spin orientations.

Indeed, the high temperature expression for x, whose definition is given by formula (6), is :

$$x = \frac{H^2}{(m+2)T^2 - m} + 0(H^4), \quad (20)$$

and has a pole at

$$T = T^* = \sqrt{\frac{m}{m+2}}.$$

However, below $T_c = 1$, the parameter q becomes finite and, to first order in q, the denominator D_0 in (20) is correspondingly modified into :

$$D = (m+2)T^2 - m + \frac{2m^2 q}{T^2(m+2)}. \quad (21)$$

To first order in $\tau = 1 - T$,

$$D_0 = 2[1 - \tau(m+2)] + 0(\tau^2), \quad (22)$$

whereas

$$D = 2\left[1 - \frac{4(m+1)}{m+2}\tau\right] + 0(\tau^2). \quad (23)$$

One observes that a finite value for q, due to the spin glass instability, has a stabilizing influence, and tends to remove the second instability, at this level of perturbation expansion in τ.

We reemphasize that, in this domain of the phase diagram, our expression for the free energy may have at best the significance of a metastable free energy (due to replica-symmetry breaking). But the mere possibility for the existence of such an unexpected phase transition calls for careful theoretical and experimental analyses. According to formulae (12), (13), (14), the hallmark for such a transition would be the onset of an anisotropy in the zero-field susceptibility.

6. **Discussion.** — All the results presented above pertain to the case $J_0 = 0$, i. e. equal probability for positive and negative values of the exchange interaction. As shown in reference [2], the generalization to finite values of J_0 is immediate. The various transition lines found in the plane (H, T) for $J_0 = 0$ give rise to transition surfaces in the phase diagram (H, T, J_0). In particular, we predict the existence of two, perhaps three, mixed phases with both ferromagnetic and spin glass characters, for sufficiently large values of a mean ferromagnetic interaction.

As a conclusion, we hope to have convinced that the infinite-ranged model of spin glasses contains a rich physics.

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