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Non-homogeneous mean field picture for spin-glasses

H. Orland, C. de Dominicis and T. Garel (*)

DPh-T, CEN Saclay, B.P. nº 2, 91190 Gif sur Yvette, France

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Résumé. — Dans cette lettre, nous calculons la moyenne gelée (sans répliques) pour des verres de spin avec désordre local. Ceci permet une définition naturelle du champ moyen. On montre que les champs moyens décrivant les verres de spin sont du type instanton.

Abstract. — In this letter we perform quenched averages (without replicas) for spin-glass systems with local disorder. This allows a natural definition of a mean field theory. The mean fields relevant to spin-glasses are shown to be instantons.

1. Introduction. — In order to explain the puzzling experimental properties of spin-glasses [1], many ingredients are likely to be necessary. On the theoretical side [2], there is wide agreement on the minimum input needed to understand *qualitatively* such properties. Namely, one should consider models with competing magnetic interactions (frustration) and quenched disorder. Most theoretical models thus replace the original problem (randomly located spins) by a lattice problem with random couplings.

Along these lines, there have been mainly two ways of approaching the delicate spin-glass problem. On the one hand, a mean field theory has been proposed by Sherrington and Kirkpatrick (SK) [3], for a model with long-range interactions; such a model displays a phase transition towards a spin-glass phase, but the presence of a quenched disorder has made so far the low temperature phase difficult to study (and to understand) [4]. Moreover, due to its mean field character, the SK model washes out all spatial correlations, and its results are expected to be relevant only for dimensions greater than six. On the other hand, computer studies for « more realistic models » (e.g. three-dimensional systems with nearest neighbour interactions) have shown that spatial correlations are important indeed [5] and some experimental results have been successfully explained in terms of a cluster picture [6]. This cluster interpretation is somewhat reminiscent of the Néel's theory of « grains fins » [7], but it seems difficult to bridge

the gap between the phase transition approach, where one expects a collective behaviour of the spins, and the cluster approach with strong intracluster couplings and weak intercluster couplings.

In this note, we wish to study a class of spin systems, with purely local disorder. For such systems, we perform in section 2, the quenched average and calculate the free energy (without replicas). A quenched partition function is defined (section 3) whose leading term is a mean density quenched free energy. Mean field theory follows from a saddle point treatment of the leading term only. In section 4, we consider two simple one-dimensional examples, namely randomly located spins interacting via long-range oscillatory interactions. The salient features of such models is the existence of non-homogeneous mean field solutions. The first example [8] displays oscillatory solutions, and is unlikely to depict a spin-glass phase whereas in the second one, clusters of spins (or instantons) show up below the transition temperature.

2. Quenched averages. — We consider a model with local disorder : N magnetic impurities are located at random sites of a D-dimensional lattice. Any of the Ω sites of the lattice can be occupied by 0 or 1 impurity. A given configuration of impurities is defined by occupation numbers n_j , taking the value 0 or 1, with the constraint :

$$\sum_{j=1}^{\Omega} n_j = N \,. \tag{1}$$

15 février **1981**, page L-73

^(*) Laboratoire de Physique des Solides, Orsay.

The partition function for such a configuration reads :

$$Z(\{n_j\}) = \frac{1}{2^{\Omega - N}} \sum_{\{S_j\}} \exp\left(\frac{\beta}{2} \sum_{j=1}^{\Omega} \sum_{l=1}^{\Omega} n_j S_j J_{jl} n_l S_l\right)$$
(2)

where the summation runs over all possible spin configurations, and J_{jl} denotes the exchange interaction between spins at sites j and l (for a realistic system, J_{jl} can be thought of as the RKKY interaction). The quenched free energy for such a system is defined by :

$$\overline{F} = -T \frac{\sum_{n_1=0,1} \cdots \sum_{n_{\Omega}=0,1} \delta\left(\sum_{j=1}^{\Omega} n_j - N\right) \operatorname{Ln} Z(\{n_j\})}{\sum_{n_1=0,1} \cdots \sum_{n_{\Omega}=0,1} \delta\left(\sum_{j=1}^{\Omega} n_j - N\right)}.$$
(3)

For Ising spins, for instance, (2) can be rewritten :

$$Z(\lbrace n_j \rbrace) = \int \prod_{j=1}^{\Omega} dm_j d\varphi_j \exp\left\{\sum_{j=1}^{\Omega} (im_j \varphi_j + n_j \ln 2 \cosh i\varphi_j) + \frac{\beta}{2} \sum_{j=1}^{\Omega} \sum_{l=1}^{\Omega} m_j J_{jl} m_l\right\}.$$
 (4)

The quenched free energy \overline{F} is thus replaced by :

$$-\overline{F} = \frac{\int_{+\infty}^{-\infty} d\alpha \prod_{j=1}^{\Omega} dn_j dv_j \exp\left(-i\alpha N + \sum_{j=1}^{\Omega} \left(in_j(\alpha + v_j) + \ln\cosh\frac{iv_j}{2} - \frac{iv_j}{2}\right)\right) \ln Z(\{n_j\})}{\int_{-\infty}^{+\infty} d\alpha \prod_{j=1}^{\Omega} dn_j dv_j \exp\left(i\alpha N + \sum_{j=1}^{\Omega} \left(in_j(\alpha + v_j) - \frac{iv_j}{2} + \ln\cosh\frac{iv_j}{2}\right)\right)}.$$
 (5)

Since Ln $Z(\{n_j\})$ behaves at most (for a given configuration) like N^2 , we may compute (5) by saddle point expansion on α , v_j , n_j around the saddle point value :

$$\sum_{j=1}^{\Omega} n_j^s = N \tag{6a}$$

$$\alpha^{\rm s} + v_j^{\rm s} = 0 \tag{6b}$$

$$n_j^{\rm s} + \frac{1}{2} \left(\tanh \frac{iv_j^{\rm s}}{2} - 1 \right) = 0$$
 (6c)

i.e.

$$n_j^{\rm s} = \frac{N}{\Omega} \equiv \rho \ . \tag{7}$$

The quenched free energy averaged over disorder, is thus given by :

$$-\frac{\overline{F}}{T} = \operatorname{Ln} Z \{ n_j \equiv \rho \} + \Delta$$
(8)

where the first term is a mean density quenched free energy and Δ stands for all corrections to this saddle point result.

This is to be contrasted with the *annealed* case where one is averaging the partition function $Z \{n_j\}$ (instead of the free energy). In that case the partition function enters the saddle point equations and (6b) is to be replaced by :

$$i(\alpha^{s} + v_{j}^{s}) + \frac{\partial}{\partial n_{j}^{s}} \operatorname{Ln} Z \{ n_{j}^{s} \} = 0 , \qquad (9)$$

leading to a solution distinct from (7).

If one expands the n_j 's around their saddle point value ρ , one obtains after resummation the full expression

L-74

for the corrections to the mean density quenched free energy,

$$\Delta = \sum_{j=1}^{N} \left[(1-\rho) \operatorname{Ln} \langle \exp[-\rho \operatorname{Ln} \cosh \varphi_{j}] \rangle_{\rho} + \rho \operatorname{Ln} \langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{j}] \rangle_{\rho} \right] + \\
+ \frac{1}{2} \sum_{j\neq i}^{N} \left[(1-\rho)^{2} \left[\operatorname{Ln} \langle \exp[-\rho (\operatorname{Ln} \cosh \varphi_{j} + \operatorname{Ln} \cosh \varphi_{i})] \rangle_{\rho} / \langle \exp[-\rho \operatorname{Ln} \cosh \varphi_{j}] \rangle_{\rho} \right] \\
\times \langle \exp[-\rho \operatorname{Ln} \cosh \varphi_{i}] \rangle_{\rho} \right] \\
+ \rho (1-\rho) \left[\operatorname{Ln}[\langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{j} - \rho \operatorname{Ln} \cosh \varphi_{i}] \rangle_{\rho} / \langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{j}] \rangle_{\rho} \\
\times \langle \exp[-\rho \operatorname{Ln} \cosh \varphi_{i}] \rangle_{\rho} \right] + j \leftrightarrow l \right] \\
+ \rho^{2} \left[\operatorname{Ln}[\langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{j} + \operatorname{Ln} \cosh \varphi_{i}]] \rangle_{\rho} / \langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{j}] \rangle_{\rho} \\
\times \langle \exp[(1-\rho) \operatorname{Ln} \cosh \varphi_{i}] \rangle_{\rho} \right] + \cdots .$$
(10)

This expression includes fluctuation effects around ρ and is valid as Ω , $N \to \infty$ with $N/\Omega \equiv \rho$. Here the average $\langle \rangle_{\rho}$ means that one uses a density matrix $\simeq \exp L \{ n_j = \rho \}$ as appearing in (4) with $n_j = \rho$.

3. Mean field theory. — In the following we shall be interested in systems with large effective number of interacting neighbours, a case relevant for « longrange » forces (or high dimensionality). In such circumstances a very good approximation is provided by the mean field theory that replaces a density matrix proportional to exp $L(\rho)$ as in (4) by a separable one $\prod \exp L_j(\rho)$:

$$L_j(\rho) \equiv -im_j \varphi_j + \rho \operatorname{Ln} 2 \cosh i\varphi_j + \phi_j m_j. \quad (11)$$

Here ϕ_j is chosen self consistently as the best possible mean field, and this is provided by the saddle point equation on $L(\rho)$:

$$m_i^{\rm s} = \tanh i\varphi_i^{\rm s} \tag{12a}$$

$$i\varphi_j^{\rm s} \equiv \phi_j = \beta \rho \sum_l J_{jl} m_l^{\rm s}$$
(12b)

yielding

$$\tanh^{-1} m_j^{\rm s} = \beta \rho \sum_l J_{jl} m_l^{\rm s} \,. \tag{13}$$

It is of interest to notice that in this mean field approximation all corrections Δ to the mean density quenched free energy vanish :

$$\Delta_{\mathbf{m},\mathbf{f}_{\star}} = 0. \tag{14}$$

Furthermore it can be shown that Δ does not either affect stability boundaries of the mean field approximation.

4. **Examples.** — To work out examples conveniently, we go to the continuous limit Ω , $N \to \infty$ and $\sum_{j}^{\Omega} \rightarrow \int_{\Omega} dx, J_{jl} \to J(x, y)$, etc....

4.1 SEPARABLE INTERACTION. — We consider a one-dimensional model with :

$$J(x, y) = \frac{J}{N} \cos k(x - y) .$$
 (15)

This model has been previously considered [8]. The mean field approximation is exact and shows a phase transition. Below T_c ($T_c = J/2$), equation (13) yields :

$$m(x) = \tanh \beta J(A \cos kx + B \sin kx)$$
(16)

where :

$$A = \int_0^\Omega \frac{\mathrm{d}y}{\Omega} m(y) \cos ky \qquad (16a)$$

$$B = \int_0^\Omega \frac{\mathrm{d}y}{\Omega} m(y) \sin ky \,. \tag{16b}$$

The periodic solution displayed in equation (16) does not seem to correspond to any realistic spinglass model (existence of long-range order).

4.2 NON-SEPARABLE INTERACTION. — We now consider a one-dimensional model with :

$$J(x, y) = J \sin k | x - y | e^{-\gamma |x - y|}$$
(17)

where $\gamma \ll k$ (which means that the oscillation period is small compared to the interaction range).

Even though this model is unlikely to show a phase transition in one dimension, mean field theory provides, as usual, a qualitative understanding of the low temperature phase in higher dimensions.

The Fourier transform of J(x, y) can be split into two terms

$$J(q) = J_1(q) + J_2(q)$$
(18)

where :

$$_{1}(q) = \frac{-Jk}{(q+i\gamma)^{2}-k^{2}}$$
 (19a)

$$J_2(q) = \frac{-Jk}{(q - i\gamma)^2 - k^2}.$$
 (19b)

Defining the functions ψ , ψ_1 , and ψ_2 by :

J

$$\psi(x) = \tanh^{-1} m(x) \tag{20a}$$

$$\psi_1(x) = \beta \rho \int_{\Omega} dy J_1(x, y) \tanh \psi(y) \quad (20b)$$

$$\psi_2(x) = \beta \rho \int_{\Omega}^{r} dy J_2(x, y) \tanh \psi(y) \quad (20c)$$

equation (13) becomes :

$$\psi(x) = \psi_1(x) + \psi_2(x)$$
(21)

or, equivalently :

$$\left(\frac{\partial^2}{\partial x^2} + \gamma^2 + k^2\right)\psi(x) - 2\gamma\frac{\partial U}{\partial x} =$$
$$= 2\beta J\rho k \tanh\psi(x) \quad (22a)$$

$$\left(\frac{\partial^2}{\partial x^2} + \gamma^2 + k^2\right) U(x) - 2\gamma \frac{\partial \psi}{\partial x} = 0 \quad (22b)$$

where :

$$U(x) = \psi_1(x) - \psi_2(x) .$$
 (23)

In the long-range approximation $(\gamma \ll k)$, equation (22b) shows that U(x) is of order γ .

Neglecting terms of order γ^2 in (22*a*), we replace equations (22) by :

$$\left(\frac{\partial^2}{\partial x^2} + k^2\right)\psi(x) = 2\ \beta J\rho k\ \tanh\psi(x)\ . \quad (24a)$$

Note that, since the function $\psi(x)$ is only defined on the length Ω , the above results were obtained with the underlying assumption that $\psi(x)$ is periodic :

$$\psi(\Omega) = \psi(0) . \tag{24b}$$

Equation (24a) is equivalent to the motion of a classical particle of mass unity in the potential :

$$V(\psi) = \frac{k^2}{2} \psi^2 - 2 \beta J \rho k \operatorname{Ln} \cosh \psi . \qquad (25)$$

A phase transition appears when the curvature of the potential at $\psi = 0$, changes sign (Fig. 1), namely, at a temperature :

$$T_{\rm c} = 2 \, \frac{J\rho}{k} \,. \tag{26}$$



Fig. 1. — Schematic potential $V(\psi)$.

At $T > T_c$, the simplest solution to equations (24) is $\psi = 0$, namely a paramagnetic phase.

Below $T_{\rm c}$, two types of solution appear :

- Homogeneous : they correspond to the two ferromagnetic phases $\psi = \pm \psi_0$, and to the paramagnetic one $\psi = 0$.

— Non-homogeneous : in the thermodynamic limit $(\Omega \rightarrow +\infty)$, new types of mean field are to be considered, namely those corresponding to motions close to zero energy (instantons) [9].

A simple study of the stability of the solutions shows that homogeneous solutions are unstable below T_c and that only inhomogeneous solutions of the instanton type may survive.

The physical picture arising below T_c is that of a gas of instantons. These instantons can be thought of as coherent spin clusters, with up or down magnetization. The finite size of these clusters (increasing with temperature and diverging at T_c) and the existence of a zero magnetization region between two such clusters (Fig. 2) are due to the frustration effect.



Two instantons

Fig. 2. — Instanton-anti-instanton classical solution.

One must keep in mind that these instantons are completely delocalized in space, yielding the picture of a paramagnetic gas of clusters (¹). In this approach, the EA order parameter, which builds up below T_c , measures the magnetization carried by one instanton.

Note that in the mean field approximation used here, T_c scales like ρ . However it is clear that for short-range interaction and small enough density ($\rho < \rho_P$ percolation threshold) the system will be paramagnetic at all temperatures. This phenomenon appears through the corrections to mean field.

For spin-glasses that do not have long-ranged interactions like insulating spin-glasses the above picture of an instanton gas should remain useful for densities sufficiently larger than $\rho_{\rm p}$.

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^{(&}lt;sup>1</sup>) In mean field theory, the instanton gas is non-interacting, whereas corrections to the mean field generate effective interactions.

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