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A solution of Sherrington Kirkpatrick model for Ising spin glass with physically acceptable entropy

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Résumé. — Nous examinons une théorie de champ moyen du modèle de Sherrington Kirkpatrick pour les verres de spin d'Ising. Cette solution généralise celle de Blandin *et al.* et constitue un cas limite de celle de Parisi. Bien que nous trouvions une bonne entropie, physiquement acceptable, près de la température nulle (identique à la solution de Sommers) l'examen de sa stabilité au sens de Almeida Thouless et Pytte Rudnick révèle que cette solution est *instable* en dessous de T_c .

Abstract. — We investigate a mean field theory of the Sherrington Kirkpatrick model of the Ising spin glass. This solution generalizes that of Blandin *et al.* and is a peculiar limit of Parisi's. Even though we find a well behaved, physically acceptable, entropy near zero temperature (identical to Sommer's solution) investigation of its stability in the sense of Almeida Thouless and Pytte Rudnick reveals it to be *unstable* below T_c .

1. Introduction. — Mean field theories in spin glasses can be roughly divided in two categories ; the spirit of the first one is to extremize the free energy with respect to a single (or a small number of) variational parameter(s), historically defined by Edwards and Anderson [1] (1975) as *the* order parameter. This procedure is quite similar to the one used in ordinary phase transitions, and implies that one averages out the disorder before the extremization of the free energy. The best illustration of this method is the Sherrington and Kirkpatrick [2] (1975) model, to be referred to as SK. Difficulties encountered in this approach led Thouless, Anderson and Palmer [3] (1977), hereafter referred to as TAP, to consider a second kind of *mean field* theory ; these authors extremize the free energy with respect to N variational parameters $\langle S_i \rangle$ (where N is the number of sites and $\langle \rangle$ denotes thermal averaging). Apart from the case of the spherical model (Kosterlitz *et al.* [4] (1976)), the two procedures yield very different results ; this emphasizes the importance of keeping track of the disorder in the thermodynamic properties of spin glasses.

In this note, we wish to present a mean field theory of the first kind. We use a scheme generalizing that of Blandin *et al.* [5] (1979) which is also a limiting

case of a symmetry breaking considered by G. Parisi [7] (1979). This scheme, which relies on replica theory, is described in section 2. Section 3 deals with the thermodynamics of the model ; in particular, we will show that the entropy is *well*-behaved when $T \rightarrow 0$. The stability of the solution, in the sense of de Almeida and Thouless [6] (1978) is investigated in section 4. We will conclude by some remarks on this type of mean field theory.

2. The model. — We consider Ising spins interacting with random Gaussian infinite-ranged interactions J_{ij} . The approach of Blandin *et al.* [5] (1979), that we briefly recall, distinguishes two essential steps :

(i) The Edwards and Anderson order parameter q is defined by introducing two replicas s_i and σ_i at each site i , interacting with the following Hamiltonian :

$$-\beta\mathcal{H} = \beta \sum_{(ij)} J_{ij}(\sigma_i \sigma_j + s_i s_j) + K \sum_i s_i \sigma_i.$$

Here K is a fictitious coupling field and one has :

$$q = \overline{\langle s_i \sigma_i \rangle} = \lim_{K \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial}{\partial K} \overline{(\text{Log Tr } e^{-\beta\mathcal{H}})}$$

where the upper bar means average over the J_{ij} .

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(ii) As usual, the calculation of the free energy is performed using the replica trick. That is, one replicates m times the initial two replica systems, and this yields $n = 2m$ replicas s_i^α and σ_i^α ($\alpha = 1 \dots m$). The Edwards and Anderson order parameter can then be defined by

$$q = \overline{\langle s_i^\alpha \sigma_i^\alpha \rangle}$$

but the replication procedure leads one to consider also two other parameters defined as :

$$\begin{aligned} r_1 &= \overline{\langle s_i^\alpha \sigma_i^\beta \rangle} & \alpha \neq \beta \\ r_2 &= \overline{\langle s_i^\alpha s_i^\beta \rangle} = \overline{\langle \sigma_i^\alpha \sigma_i^\beta \rangle} & \alpha \neq \beta. \end{aligned}$$

As shown in detail by Blandin *et al.* [5] (1979), the extremization of the free energy is consistent with the choice $r_1 = r_2 = r$. This choice yields at zero temperature the same energy as SK and an entropy which is half their result.

We now extend the model, as in G. Parisi [1] (1979) by taking, not only two replicas as above, but p replicas on each site denoted by $s_i^\alpha, s_i^{\alpha'}, s_i^{\alpha''} \dots$. Replicating the system m times (as above α becomes in turn $\alpha, \beta, \gamma \dots$) we get $n = pm$ replicas. The order parameter is now defined as :

$$q = \overline{\langle s_i^\alpha s_i^{\alpha'} \rangle} \quad (\alpha') \neq \alpha$$

where (α') denotes any value of the line $\alpha, \alpha', \alpha'' \dots$. The other parameter is defined as

$$r = \overline{\langle s_i^\alpha s_i^\beta \rangle} \quad \beta \neq (\alpha').$$

Note that this is the minimal procedure to break the symmetry between replicas ; one could think as well of introducing more parameters, for simplicity, we will restrict ourselves to q and r .

3. Thermodynamic properties. — The calculation of the free energy is exactly the same as in SK [2] with the result :

$$\begin{aligned} -\frac{F(p)}{NT} &= \frac{\tilde{J}^2}{4T^2} [p(r-1)^2 + (1-p)(q-1)^2 - 2p(q-r)] + \\ &+ \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{p} \text{Ln} \left[\int_{-\infty}^{+\infty} \frac{dy}{\sqrt{2\pi}} e^{-y^2/2} e^{p \text{Ln} 2 \text{ch} B} \right] \end{aligned} \quad (1)$$

with

$$B = y(Q - R)^{1/2} + xR^{1/2},$$

and where $\tilde{J}/\sqrt{N}$ is the variance of the J_{ij} distribution and

$$Q = \frac{\tilde{J}^2}{T^2} q, \quad R = \frac{\tilde{J}^2}{T^2} r.$$

Straightforward calculations show that the zero temperature entropy and energy write

$$\begin{aligned} S^0(p) &= \frac{S_0}{p} \\ E^0(p) &= E_0, \end{aligned}$$

where S_0 and E_0 are SK's results.

Considering the fact that S_0 is negative, we choose *a priori* $p = \infty$. The important point in this respect is to note that the quantity $a = p(q - r)$ remains finite when $p = \infty$.

Setting $A = \frac{\tilde{J}^2}{T^2} a = p(Q - R)$, we perform a

saddle point integration under the Ln sign of Eq. (1) which is *exact* in the $p = \infty$ limit. In terms of the order parameters a and r we get :

$$\begin{aligned} -\frac{F(\infty)}{NT} &= \frac{\tilde{J}^2}{4T^2} [(r-1)^2 - 2ar] + \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \times \\ &\times \left[-\frac{1}{2} \frac{Y_0^2}{A} + \text{Ln} 2 \text{ch} (Y_0 + xR^{1/2}) \right] \end{aligned} \quad (2)$$

where $Y_0 \equiv Y_0(x, A, R) = A \text{th} (Y_0 + xR^{1/2})$ corresponds to the saddle point.

Extremizing (2) with respect to a and r , we have :

$$R^{1/2}(r-1-a) = - \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} x \text{th} (Y_0 + xR^{1/2}) \quad (3)$$

$$r = \int_{-\infty}^{+\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \text{th}^2 (Y_0 + xR^{1/2}). \quad (4)$$

Eqs. (3) and (4) can be easily studied around $T = T_c (= \tilde{J})$ and at low temperatures with the following results :

(i) $T \simeq T_c$

$$r = t + \frac{5}{3} t^2 + O(t^3) \quad (5)$$

$$a = \frac{4}{3} t^2 + O(t^3) \quad (6)$$

where $t = \left(\frac{T_c - T}{T_c} \right)$.

(ii) $T \simeq 0$ — To leading order, we have :

$$r = 1 - \frac{4}{\sqrt{2\pi}} \frac{T}{\tilde{J}} e^{-2a(\tilde{J}^2/T^2)} \quad (7)$$

$$a = \frac{2}{\sqrt{2\pi}} \frac{T}{\tilde{J}} \quad (8)$$

which gives

$$-\frac{F^0(\infty)}{NT} = \sqrt{\frac{2}{\pi}} \frac{\tilde{J}}{T} + \frac{1}{\sqrt{2\pi}} \frac{T}{\tilde{J}} \exp \left(-\frac{4}{\sqrt{2\pi}} \frac{\tilde{J}}{T} \right). \quad (9)$$

This in turn yields

$$E^0(\infty) = -\sqrt{\frac{2}{\pi}} \mathcal{J} = E_0 \quad (10)$$

$$S^0(\infty) = \frac{4}{2\pi} \exp \left[-\frac{4}{\sqrt{2}\pi} \left(\frac{\tilde{\mathcal{J}}}{T} \right) \right]. \quad (11)$$

The entropy is therefore well-behaved as $T \rightarrow 0$ and, in this model, the Ising character of the spins is transparent, in contrast with the TAP results showing a power law behaviour of the entropy as $T \rightarrow 0$. Note that the entropy is the same as that found by Sommers [8] (1978) in a different context.

4. Stability of the solution. — The fact that the SK solution, which preserves the symmetry between replicas, yields a negative entropy at low temperatures can be linked to an unstability of this solution below T_c , as shown by de Almeida and Thouless [6] (1978)

and Pytte and Rudnick [9] (1979). These authors expand to second order the free energy around the SK solution, and therefore break the symmetry between replicas. Having obtained a well-behaved entropy with the solution of section 3, it is therefore of interest to study the stability of this solution against further symmetry breaking. Defining

$$\begin{aligned} \overline{\langle s_i^\alpha s_i^{\alpha'} \rangle} &= q + \eta^{\alpha\alpha'} \\ \overline{\langle s_i^\alpha s_i^\beta \rangle} &= r + \eta^{\alpha\beta} \quad \beta \neq \alpha' \end{aligned}$$

the quadratic form of interest reads, in matrix notation :

$$\mathcal{H}_2 = \frac{1}{2} \boldsymbol{\eta} \mathbf{G} \boldsymbol{\eta}$$

where :

$\boldsymbol{\eta}$ is the vector of components $(\eta^{\alpha\beta})$,

$\mathbf{G}$ is defined with the help of the following four matrices.

(i) The identity matrix $\mathbf{1}$

$$\mathbf{1}_{(\alpha\beta)(\gamma\delta)} = \begin{cases} 1 & \text{if } (\alpha = \gamma \text{ and } \beta = \delta) \text{ or } (\alpha = \delta \text{ and } \beta = \gamma) \\ 0 & \text{otherwise.} \end{cases}$$

(ii) The association matrix $\mathbf{R}$

$$\mathbf{R}_{(\alpha\beta)(\gamma\delta)} = \begin{cases} 1 & \text{if } (\alpha = \gamma, \beta \neq \delta) \text{ or } (\alpha = \delta, \beta \neq \gamma) \text{ or } (\alpha \neq \gamma, \beta = \delta) \text{ or } (\alpha \neq \delta, \beta = \gamma) \\ 0 & \text{otherwise.} \end{cases}$$

(iii) The matrix $\mathbf{S}$

$$\mathbf{S}_{(\alpha\beta)(\gamma\delta)} = \begin{cases} 0 & \text{if } (\alpha = \gamma, \beta = \delta) \text{ or } (\alpha = \delta, \beta = \gamma) \\ 1 & \text{otherwise.} \end{cases}$$

(iv) The matrix $\boldsymbol{\rho}$

$$\boldsymbol{\rho}_{(\alpha\beta)(\gamma\delta)} = \begin{cases} 1 & \text{if } (\alpha = \gamma, \beta = \delta') \text{ or } (\alpha = \delta, \beta = \gamma') \text{ or } (\beta = \gamma, \alpha = \delta') \text{ or } (\beta = \delta, \alpha = \gamma') \\ 0 & \text{otherwise.} \end{cases}$$

We recall that by α' , we denote one of the $(p-1)$ replicas belonging to the line (α) (and different from α). We note that the matrix $\boldsymbol{\rho}$ does *not* commute with $\mathbf{R}$ and $\mathbf{S}$.

The matrix $\mathbf{G}$ can then be expressed as :

$$\mathbf{G} = D\mathbf{1} + (B - C)\mathbf{R} + C\mathbf{S} - \frac{a}{p}\boldsymbol{\rho}, \quad (12)$$

and recall that we are interested in the limit $p = \infty$. Here, we have

$$D = \left(\frac{T}{\mathcal{J}} \right)^2 - 1 \quad (13)$$

$$B = -r = - \int \text{th}^2(Y_0 + xR^{1/2}) \frac{dx}{\sqrt{2}\pi} e^{-x^2/2} \quad (14)$$

$$C = - \int \text{th}^4(Y_0 + xR^{1/2}) \frac{dx}{\sqrt{2}\pi} e^{-x^2/2}. \quad (15)$$

In what follows, we restrict ourselves to the vicinity of T_c , that is we take

$$r = t + \frac{5}{3}t^2 + O(t^3)$$

$$a = \frac{4}{3}t^2 + O(t^3).$$

Due to the fact that $\boldsymbol{\rho}$ does not commute with $\mathbf{R}$ and $\mathbf{S}$, the search for the eigenvectors and eigenvalues

of the form (5) is rather tedious, and we just quote the results. There are five eigenvalues :

$$\begin{aligned}\mu_1 &= \mu_2 = D - 2B + C = \frac{4}{3} t^2 \\ \mu_3 &= \mu_4 = D - 4B + 3C - 4a = 2t + O(t^2) \\ \mu_5 &= D - 2B + C - 2a = -\frac{4}{3} t^2.\end{aligned}$$

The instability shows up in μ_5 , with precisely the same coefficient as in de Almeida and Thouless (1978). In their case, however, there are only three eigenvalues and the instability is associated with μ_1 . The stability of the solution of Blandin *et al.* (1979) which corresponds to $p = 2$ gives the same results as the case $p = \infty$. We are therefore forced to conclude that the solution of section 3 is unstable, even though its entropy is positive, i.e. physically acceptable.

5. Conclusions. — The instability of the SK solution, as found by de Almeida and Thouless (1978) was linked to the appearance of a negative entropy at low temperature. We have tried to mend the replica theory of SK using a peculiar symmetry breaking. The results show that one can find a physically

acceptable entropy but the solution still contains a negative mass in its spectrum. Thus the steepest descent expansion that is associated with mean field approximations and of which it is the zeroth order (tree resummation) blows up at next order.

Whether *any* conceivable symmetry breaking with a finite number of order parameters will be able to provide a satisfactory solution and bring the entropy from $S \sim \exp(-c/T)$ as $T \rightarrow 0$, to the TAP result in $S \sim T^2$ is yet unknown. The T^2 law seems to be linked to the presence of massless modes in the Ising spin glass as suggested by Bray and Moore [10], whereas the behavior obtained is suggestive of a gap.

We wish to thank A. Blandin for fruitful discussions.

NOTE. — As this manuscript was completed we received a very interesting preprint by Bray and Moore [11] where they also derive the result of section 3. Besides they prove the equivalence of Eqs. (2)-(4) with the result of Sommers [8], thus making a connection between the type of symmetry breaking with $p \rightarrow \infty$ and a simple approximation of TAP equations.

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