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What is the static Edwards-Anderson order parameter in the mean-field theory of spin glasses ?

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Résumé. — Nous présentons une preuve, par la méthode des répliques, de la proposition suivante : la valeur moyenne quadratique du spin local dans le modèle de verre de spin de Sherrington et Kirkpatrick est égale au minimum $q(0)$ des paramètres d'ordre $q(x)$ de Parisi. Ceci correspond à l'interprétation dynamique de Sompolinsky concernant $q(x)$. On montre que $q(0)$ obéit à une loi de puissance $q(0) \sim b^{2/3}$ pour de faibles champs appliqués b et pour des domaines de températures $0 < T < T_c$. De plus on calcule l'aimantation en champ faible à toutes températures. Les calculs sont basés sur une relation exacte pour la susceptibilité locale renormalisée, qui remplace l'hypothèse de Parisi et Toulouse.

Abstract. — We present a replica derivation for the claim that the averaged square of the local spin expectation value in the long-range spin glass model is equal to the minimum, $q(0)$ of Parisi's order parameters $q(x)$. This corresponds to the dynamic interpretation of $q(x)$ due to Sompolinsky. We show that $q(0)$ obeys a power law $q(0) \sim b^{2/3}$ for low external fields b and all temperatures $0 < T < T_c$. Furthermore we calculate the low field magnetization for all temperatures. The calculations are based on an exact relation for the renormalized local susceptibility which replaces the Parisi-Toulouse hypothesis.

Edwards and Anderson [1] suggested originally the time persistent part of the local spin correlation as the spin glass order parameter

$$\tilde{q} = \lim_{t \rightarrow \infty} \overline{\langle S_i S_i(t) \rangle}. \quad (1)$$

We consider for simplicity an Ising model ($S_i = \pm 1$). The bar denotes the configuration average with respect to the random exchange interactions and the brackets denote the thermal or dynamical average. In the mean-field approximation made by Edwards and Anderson and Sherrington and Kirkpatrick [2] $\tilde{q}$ was replaced by the static Edwards-Anderson order parameter

$$q = \overline{\langle S_i \rangle^2}. \quad (2)$$

Edwards and Anderson implicitly assumed the equivalence of both definitions since for very long times the dynamical correlations should decay. $\tilde{q}$ is the order parameter which can be calculated by Monte-Carlo computer simulations [3]. Unfortunately the definition (1) seems to be

ill-defined for long-range spin glasses. Sompolinsky [4] suggested a continuum of order parameters

$$q(x) = \overline{\langle S_i S_i(\tau_x) \rangle} \quad (3)$$

where τ_x are relaxation times arranged in a decreasing order ($0 \leq x \leq 1$) which all go to infinity in the thermodynamic limit but $q(x)$ remains a monotonous function between 0 and 1. Sompolinsky introduced a second order parameter $\Delta(x)$ where $\beta(1 - q(1) + \Delta(x))$ is the local susceptibility on a time scale τ_x . He derived, with the help of certain assumptions, a selfconsistent theory which turned out to be equivalent to the theory of Parisi [5] with $\Delta'(x) = -xq'(x)$ subject to $-\Delta'(x)/q'(x)$ being monotonic. However in the Parisi theory the definition of x is slightly different so that $q(x)$ is constant outside a certain interval where it increases monotonically. The definition of the boundary values is invariant. Thus we have two well defined limits $q(0)$ and $q(1)$. It was suggested [6, 7] that $q(1)$ is equal to q since this accounts well for the results of computer simulations [8]. However, it has been pointed out by Young and Kirkpatrick ([9], hereafter referred to as YK) that this interpretation is wrong since they determined numerically an inequality for the internal energy per spin, u ,

$$-\beta u \leq \frac{(\beta J)^2}{2} (1 - q^2) \quad (4)$$

which is violated by the Parisi-Sompolinsky solution if $q = q(1)$, since $\Delta'(x) < 0$.

We are considering an Ising model of N interacting spins in external fields b_i with the Hamiltonian

$$H = - \sum_{i < j} J_{ij} S_i S_j - \sum_i b_i S_i \quad (5)$$

where the long-range interactions have the distribution

$$P[J_{ij}] \propto \exp\left(-\frac{1}{2} \sum_{i < j} J_{ij}^2 N/J^2\right). \quad (6)$$

Inequality (4) can be proved rigorously following Bray and Moore [10]

$$\begin{aligned} -\beta u &= \frac{1}{2N} \sum_{i \neq j} \overline{\beta J_{ij} \langle S_i S_j \rangle} \\ &= \frac{(\beta J)^2}{2N^2} \sum_{ij} (1 - \overline{\langle S_i S_j \rangle^2}) \leq \frac{(\beta J)^2}{2} \left(1 - \left(\frac{1}{N} \sum_i \overline{\langle S_i \rangle^2}\right)^2\right). \end{aligned} \quad (7)$$

The second equality follows by partial integration, the inequality follows decomposing $\langle S_i S_j \rangle$ into $\chi_{ij} + \langle S_i \rangle \langle S_j \rangle$ and using the positivity of the matrix χ_{ij} and of $\left(\sum_i (\langle S_i \rangle^2 - \overline{\langle S_i \rangle^2})\right)^2$.

According to the theory of Sompolinsky $q(1)$ is the quantity that is calculated in computer simulations and $q = q(0)$. The last claim has never been written down but it is the natural consequence of Sompolinsky's theory. We present below a replica derivation of this statement which also reflects why the replica derivation of the local susceptibility does not give the result which is obtained for finite N by varying only the one local field at the site considered. The replica derivation gives the renormalized local susceptibility discussed below.

YK claimed that q cannot be simply expressed by $q(x)$. However they calculated q using a restricted ensemble of spins having a positive projection onto the magnetization, since then q as function of the external field b extrapolates linearly to a finite value for $b \rightarrow 0$. However,

there exist many possibilities of such restricted ensembles which all give different results for $b \rightarrow 0$ (a few have been presented by YK). They seem to correspond to the different relaxation times of Sompolinsky. The linear extrapolation for $b \rightarrow 0$ may correspond to a certain $q(x)$. One calculation of YK without restriction is well compatible with a power law dependence of q for $b \rightarrow 0$. It shows that the linear extrapolation calculated with the restricted ensemble mentioned above starts at a field which is an order of magnitude greater than the field where the magnetization rapidly goes to zero. We will show below that $q(0)$ has a power law dependence

$$q(0) \propto b^{2/3} \quad (8)$$

for all temperatures $T > 0$ below the critical temperature T_c . This has been shown by Parisi [6] for $T \rightarrow T_c$. Besides it follows that $q(0) = 0$ for $b = 0$ which coincides with the result of Morgenstern and Binder in two and three dimensions [11]. Thus the spin glass phase is critical for all temperatures $0 < T < T_c$. The above critical index is universal and temperature independent. Sompolinsky and Zippelius [12] obtained a temperature dependent critical index for the low frequency behaviour of the dynamical spin correlation. However, the connection of the dynamical theory with the full equilibrium theory is not quite clear because of the ill-defined limits for $t \rightarrow \infty$ (Eq. (1)). The above critical index (Eq. (8)) is based on an exact relation for the renormalized local susceptibility which is valid for all temperatures and external fields in the spin glass phase and has been derived by the author from the Sompolinsky equations. It replaces the Parisi-Toulouse hypothesis [13] and the Bray-Moore criterion for a soft mode [14]. Furthermore we calculate the magnetization and susceptibility for low fields and explain the difference between local susceptibility, renormalized local susceptibility and total susceptibility.

We start with a replica derivation of $q = q(0)$. The replica method consists of averaging $\text{Tr } W^n$ with a positive integer n and $W = \exp(-\beta H)$ and trying to obtain $\overline{\log \text{Tr } W}$ from the continuation $n \rightarrow 0$. We may also directly calculate derivatives of the free energy by the replica method. A crucial point is that $\text{Tr } W^n$ can be written as an integral over variables $q_{\alpha\beta}$, $0 < \alpha < \beta \leq n$, which can be evaluated for $N \rightarrow \infty$ by saddle point integration. Let us divide the n replicas $\{\alpha\}$ into two groups $\{\alpha_1\}$, $\{\alpha_2\}$ with n_1 , n_2 replicas

$$W^n = W^{n_1} \cdot W^{n_2}. \quad (9)$$

Assume now that the local external field $b_i^{(1)}$ in the first group is different from the field $b_i^{(2)}$ in the second group. Then

$$\begin{aligned} \frac{\partial}{\partial \beta b_i^{(1)}} \cdot \frac{\partial}{\partial \beta b_i^{(2)}} \text{Tr } W^n &= n_1 \langle S_i \rangle_1 \cdot n_2 \langle S_i \rangle_2 \text{Tr } W^n \\ &= \sum_{\alpha_1 \alpha_2} \text{Tr } W^n S_i^{\alpha_1} S_i^{\alpha_2}. \end{aligned} \quad (10)$$

The index α or α_1 , α_2 indicates which replica the spin S_i^α belongs to. $\langle S_i \rangle_1$, $\langle S_i \rangle_2$ mean the expectation values in the fields $b_i^{(1)}$, $b_i^{(2)}$, respectively. The traces should be normalized so that $\text{Tr } 1 = 1$. W^n in equation (10) means actually $W_1^{n_1} \cdot W_2^{n_2}$ with different fields in the two groups. We have explicitly used the fact that $b_i^{(1)}$ is independent of α_1 and $b_i^{(2)}$ is independent of α_2 . Thus $\text{Tr } W^n S_i^{\alpha_1} S_i^{\alpha_2}$ is a constant.

Now we have to average and to take the limit $n \rightarrow 0$. From equation (10) we get

$$\begin{aligned} \overline{\langle S_i \rangle^2} &= \lim_{n \rightarrow 0} \lim_{b_i^{(1)} \rightarrow b_i^{(2)}} \overline{\langle S_i \rangle_1 \langle S_i \rangle_2 \text{Tr } W^n} \\ &= \lim_{n \rightarrow 0} \lim_{b_i^{(1)} \rightarrow b_i^{(2)}} \overline{\text{Tr } W^n S_i^{\alpha_1} S_i^{\alpha_2}}. \end{aligned} \quad (11)$$

We are interested in the limit $N \rightarrow \infty$. The r.h.s. of equation (11) can be evaluated by the method of steepest descents if we interchange the limits $n \rightarrow 0$ and $N \rightarrow \infty$. This is the standard way to proceed. The result becomes proportional to the normalization factor $\text{Tr } W^n$ which goes to 1 for $n \rightarrow 0$. We use the fact that $\langle S_i \rangle^2$ is independent of i . Then it is easy to see (e.g. by the method of Ref. [7]) that the result is

$$\overline{\langle S_i \rangle^2} = q_{\alpha_1 \alpha_2} \quad (12)$$

where $q_{\alpha_1 \alpha_2}$ means the value at the stationary point. This statement is not trivial in the case of replica symmetry breaking, since equation (12) is only valid if $q_{\alpha_1 \alpha_2}$ is constant for α_1 belonging to the first group and α_2 to the second group. $q_{\alpha_1 \alpha_2}$ is not maximized as claimed by Thouless *et al.* [7]. For a system of two replicas equation (12) coincides with the order parameter definition of Blandin *et al.* [15, 16]. The two fields $b_i^{(1)}$ and $b_i^{(2)}$ have only been introduced for the partition of the replicas into two groups. Further replica symmetry breaking is produced by interchanging the limits $n \rightarrow 0$ and $N \rightarrow \infty$.

Now we look for a replica symmetry breaking solution which contains a partition such that (12) is independent of α_1 and α_2 . Furthermore $q_{\alpha_1 \alpha_2}$ should be independent of the choice of the partition if several partitions with the desired property exist. The solution should go to Parisi's solution for $b_i^{(1)} \rightarrow b_i^{(2)}$ and indeed Parisi's solution has the properties which are needed. The symmetry breaking scheme of Parisi consists in the following. The zero step is $q_{\alpha\beta} = q_0$ for $\alpha \neq \beta$. In a first step the n replicas are divided into n/m_1 groups of m_1 replicas with a new q_1 within each group as indicated in figure 1. In a next step the same procedure is applied to the q_1 matrices and so on. We see from figure 1 that the only possibility for dividing the replicas into two groups with the desired property is that n_1/m_1 and n_2/m_1 are integers. Thus we get for the Parisi solution in the limit $n \rightarrow 0$

$$\overline{\langle S_i \rangle^2} = q_0 = q(0). \quad (13)$$

In our approach the partition (n_1, n_2) is given first and then the limit $N \rightarrow \infty$ is taken, which produces the stable replica symmetry breaking scheme. Therefore the partition is not completely arbitrary if we start from Parisi's solution.

We can use the same method to find the averages of higher powers of $\langle S_i \rangle$:

$$\overline{\langle S_i \rangle^m} = \lim_{n \rightarrow 0} \text{Tr } W^n S_i^{\alpha_1} \dots S_i^{\alpha_m} \quad (14)$$

Fig. 1. — Schematic form of the matrix $q_{\alpha\beta}$ after the first iteration step of Parisi. One possible partition (n_1, n_2) into two groups with $q_{\alpha_1 \alpha_2} = q_0$ is indicated.

which must be constant with respect to $\alpha_1, \alpha_2, \dots, \alpha_m$. Again the only possibility is that the decomposition of the replicas into m groups must be commensurate with the first iteration step of Parisi. It immediately follows

$$\overline{\langle S_i \rangle^m} = \int \frac{dz}{\sqrt{2\pi}} e^{-z^2/2} m_0(\beta b + \beta J z \sqrt{q(0)})^m = \overline{m_0^m} \quad (15)$$

where $m_0(y)$ is obtained from all the next iteration steps in the same way as in Parisi's work [17]. Thus

$$m_0(y) = \frac{\partial}{\partial y} \phi(y, 0) \quad (16)$$

where $\phi(y, x)$ obeys the Parisi differential equation

$$\frac{\partial}{\partial x} \phi(y, x) = -\frac{(\beta J)^2}{2} q'(x) \left(\frac{\partial^2}{\partial y^2} \phi(y, x) + x \left(\frac{\partial}{\partial y} \phi(y, x) \right)^2 \right) \quad (17)$$

with the boundary condition

$$\phi(y, 1) = \log(2 \cosh y). \quad (18)$$

Equation (15) is similar to the Sherrington-Kirkpatrick case. The only difference is that $m_0(y) \neq \tanh y$. $m_0(y)$ is renormalized due to the interaction according to equation (17) and is thus additionally a functional of $q'(x)$.

We now derive the low field properties using a relation which has been derived by the author from the Sompolinsky equations

$$1 = (\beta J)^2 \overline{(m'_0)^2} = \overline{\left(J \frac{\partial}{\partial b} m_0 \right)^2}. \quad (19)$$

This equation is valid for all external fields and it represents the correct formulation of the Parisi-Toulouse hypothesis [13] : the averaged square of the renormalized local susceptibility is constant. It corrects also the Bray-Moore criterion for a soft mode [14]. However, one can show that an analogous equation exists for all x , for $x = 1$ it takes the form of Bray and Moore. Equation (19) follows from the selfconsistency equation for $q(x)$ differentiated with respect to x for $x \rightarrow 0$ (in the Sompolinsky formulation). A more detailed derivation will be published elsewhere. In addition we have equation (13)

$$q(0) = \overline{m_0^2}. \quad (20)$$

Expanding both equations with respect to $\beta \tilde{b} = \beta b + \beta J z \sqrt{q(0)}$ we get :

$$(\beta J)^{-2} = m'_0(0)^2 + \overline{(\beta \tilde{b})^2} m'_0(0) \cdot m_0^{(3)}(0) + \overline{(\beta \tilde{b})^4} (m_0^{(3)}(0)^2/4 + m'_0(0) \cdot m_0^{(5)}(0)/12) + \dots \quad (21)$$

and

$$q(0) = \overline{(\beta \tilde{b})^2} m'_0(0)^2 + \overline{(\beta \tilde{b})^4} m'_0(0) \cdot m_0^{(3)}(0)/3 + \overline{(\beta \tilde{b})^6} (m_0^{(3)}(0)^2/36 + m'_0(0) \cdot m_0^{(5)}(0)/60) + \dots \quad (22)$$

$q(0)$ turns out to be of order $(\beta b)^{2/3}$. We multiply equation (21) with $\overline{(\beta \tilde{b})^2}$ subtract both equations and take into account only terms up to the order $(\beta b)^2$. Performing the simple Gaussian averages we get

$$(\beta b)^2 = \frac{1}{3} (\beta J)^6 q(0)^3 \cdot m_0^{(3)}(0)^2. \quad (23)$$

In the last equation we may replace $m_0^{(3)}(0)$ by the value for $b \rightarrow 0$, i.e. neglecting the corrections of $q'(x)$ due to the external field. Thus we have proved the power law, equation (8), for all $0 < T < T_c$. The coefficient is determined by the Parisi solution for $b = 0$. For $T \rightarrow T_c$ we have

$$q(0)^3 = \frac{3}{4} \left(\frac{b}{J} \right)^2 \quad (24)$$

which coincides with the Parisi result [6].

Let us now expand the magnetization for $b \rightarrow 0$

$$\bar{m}_0 = \bar{\beta} \bar{b} m'_0(0) + \frac{(\bar{\beta} \bar{b})^3}{3!} m_0^{(3)}(0) + \frac{(\bar{\beta} \bar{b})^5}{5!} m_0^{(5)}(0) + \dots \quad (25)$$

From equation (21) we find $m'_0(0)$ up to the desired order. Introducing this into equation (25) we obtain

$$\begin{aligned} \bar{m}_0 &= \frac{b}{J} \left(1 - \frac{(\beta J)^6}{4} q(0)^2 \cdot m_0^{(3)}(0)^2 + \dots \right) \\ &= \frac{b}{J} \left(1 - \frac{3}{4} \frac{(b/J)^2}{q(0)} \right). \end{aligned} \quad (26)$$

Up to this order we find

$$\bar{m}_0 / \beta b = \bar{m}'_0. \quad (27)$$

This is the usual relation between the magnetization and the susceptibility for low fields. However, because of the singular behaviour, equation (23), this is not the total susceptibility

$$\frac{d}{db} \bar{m}_0 = \frac{1}{J} \left(1 - \frac{7}{4} \frac{(b/J)^2}{q(0)} \right). \quad (28)$$

Parisi [6] did not distinguish between the two susceptibilities. $\bar{m}'_0$ is the renormalized local susceptibility, it is the derivative of the magnetization with respect to the external field for fixed order parameters $q(0)$, $q'(x)$. Thus it does not contain the critical dependence on the magnetic field. For fixed order parameters it can be expanded in powers of the external field. On the other hand, for the total susceptibility the dependence of the order parameters on the external field is needed. The unrenormalized local susceptibility obeys a simple Curie law for $b = 0$ since $q(0) = 0$, however this is not a macroscopic thermodynamic quantity in the spin glass phase. From the replica calculation it is easily seen that

$$\bar{m}'_0 = \lim_{n \rightarrow 0} \left(1 + \frac{1}{n} \sum_{\alpha \neq \beta} q_{\alpha\beta} \right). \quad (29)$$

The above replica derivation shows that the right hand side is only equal to the unrenormalized local susceptibility, $\delta \langle S_i \rangle / \delta \beta b_i = 1 - \langle S_i \rangle^2$ if $q_{\alpha\beta}$ is constant, i.e. without replica symmetry breaking.

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