Nature of the Spin-Glass Phase

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(Received 12 December 1983)

A probability distribution has been proposed recently by one of us as an order parameter for spin-glasses. We show that this probability depends on the particular realization of the couplings even in the thermodynamic limit, and we study its distribution. We also show that the space of states has an ultrametric topology.

PACS numbers: 75.50.Kj

A lot of effort has been devoted to the understanding of the spin-glasses.[1-10] The picture which has emerged is that the main characteristic of the glassy phase is the existence of a large number (infinite when the number of spins $N \to \infty$) of equilibrium states $\alpha = 1, 2, \ldots$ (free-energy valleys separated by free-energy barriers becoming infinitely high in the thermodynamic limit).

In a recent paper[11] [to be referred to later as (I)], one of us has proposed an order parameter for the spin-glass phase and has shown its interpretation in terms of the many-valley picture. We have exploited this interpretation further and in the present Letter we present our results and their implications. Their detailed derivation will be presented elsewhere.[12]

We may characterize a pure (clustering) state α of a spin-glass by the magnetization $m_i^\alpha \equiv \langle \sigma_i \rangle_\alpha$ at each point i. (We denote the thermal averages by angular brackets and the averages over the coupling J_{ij} distribution by overbars.) As in (I) we define the overlap $q^{\alpha\beta}$ of two pure states α, β,

$$q^{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} m_i^\alpha m_i^\beta \tag{1}$$

($q^{\alpha\alpha}$ is the familiar Edwards-Anderson order parameter), and the probability $P_J(q)$ for a pair of states (α, β) to have an overlap q,

$$P_J(q) = \sum_{\alpha,\beta} P_\alpha P_\beta \delta(q - q^{\alpha\beta}), \quad \overline{P_J(q)} \equiv P(q), \tag{2}$$

where P_α, P_β are the weights of the pure states α and β. [Obviously $P_J(q) = 0$ for $q > 1$ or $q < -1$, $\int_{-1}^{1} dq\, P(q) = 1$.] We also consider the probability $Y_J(q)$ for a pair of pure states (α, β) to have an overlap bigger than q,

$$Y_J(q) = \int_q^1 dq' \, P_J(q'), \quad \overline{Y_J(q)} \equiv y(q). \tag{3}$$

The probability function $P(q)$ was proposed in (I) as the order parameter for spin-glasses and was computed in the mean-field approximation by use of the replica method.

We will show in the present note, by explicit replica-scheme calculations, that the fluctuations of $P_J(q)$ with respect to q do not vanish in the thermodynamic limit and that the appropriate order parameter for spin-glasses is the probability distribution of $P_J(q)$ [or equivalently of $Y_J(q)$]. Furthermore, we will compute the probability distribution of $Y_J(q)$. In such a way the order parameter of spin-glasses, far from being a parameter, was shown to be a function, interpreted as a probability law. And now, on top of that, there appears a probability law for this function, i.e., a probability law for a probability law. We will also show that the space of pure spin-glass states has an ultrametric topology. This means that if we take any three pure states and compute the three overlaps between them, q_1, q_2, and q_3, we will find that at least two of them (say q_1 and q_2) are equal, $q_1 = q_2$, and that the third one is bigger than or equal to them: $q_3 \geq q_1 = q_2$. This has the consequence that for any value of q, by grouping together all the pure states having overlaps bigger than q, we separate the space of pure states into disjoint clusters. Each cluster is again divided into smaller clusters by grouping together the states with overlaps bigger than $q' > q$ and so on.

The mean-field theory approximation for spin-glasses has been formulated in the context of the infinite-range model.[2] One considers n copies of the same system, averages over this coupling distribution, and, at the end, takes the limit $n \to 0$. In this way one computes averages $\overline{O_i(J)}$ of the physical observables $O_i(J)$ over the coupling distribution, hoping that in the thermodynamic limit, $O_i(J) \to \overline{O_i(J)}$.

In the replica approach, the order parameter is an $n \times n$ matrix Q_{ab}. In the limit $n \to 0$, because of replica symmetry breaking (RSB), the matrix is characterized by a function $Q(x)$,[5] where $0 \leq x \leq 1$. It was shown in (I) that $Q(x)$ is identical to $q(x)$, the inverse function of $x(q) \equiv 1 - y(q) = \int_{-1}^{q} dq' \, P(q')$, thus giving a physical interpretation to replica symmetry breaking.

We now compute the average (over the J's) probability $P(q_1,q_2,q_3)$ for any three pure states to have overlaps q_1, q_2, and q_3. The method for this computation is a straight generalization of the method in (I). We consider the generalized Laplace transform

$$q(y_1,y_2,y_3)=\int \prod_{i=1}^{3} dq_i \exp\left(\sum_{i=1}^{3} y_i q_i\right) P(q_1,q_2,q_3)$$
$$=\langle \exp\{N^{-1}\textstyle\sum_j [y_1\sigma_2(j)\sigma_3(j)+y_2\sigma_3(j)\sigma_1(j)+y_3\sigma_1(j)\sigma_2(j)]\}\rangle_3, \quad (4)$$

where $\sigma_i(j)$, $i=1,2,3$, are the spins of three identical systems and $\langle\ \rangle_3$ means the thermal average with the Hamiltonian $H=H(\sigma_1)+H(\sigma_2)+H(\sigma_3)$.

We compute $g(y_1,y_2,y_3)$ in the replica scheme by introducing, as usual, the $n\times n$ matrix Q_{ab} and taking at the end $n\to 0$:

$$q(y_1,y_2,y_3)=\lim_{n\to 0}\frac{1}{n(n-1)(n-2)} \sum_{\substack{a,b,c=1\\ a\neq b, b\neq c, c\neq a}}^{n} \exp(y_1Q_{ab}+y_2Q_{bc}+y_3Q_{ca}),$$

from which we get, after some algebra,

$$P(q_1,q_2,q_3)=\tfrac{1}{2}P(q_1)x(q_1)\delta(q_1-q_2)\delta(q_2-q_3)$$
$$+\tfrac{1}{2}\{P(q_1)P(q_2)\theta(q_1-q_2)\delta(q_2-q_3)+\text{permutations}\}. \quad (5)$$

This equation establishes the ultrametric topology of the space of pure states: Its consequence is the hierarchical organization of the space of states. Consider any three pure states α, β, and γ and their overlaps q_1, q_2, and q_3. Let us order them $q_1\geq q_2\geq q_3$. Then from Eq. (5)

$$q_1\geq q_2=q_3. \quad (6)$$

Take now any two states α and β and consider $I_\alpha(q)$ [respectively, $I_\beta(q)$] the set of pure states such that their overlaps with α (respectively, with β) are bigger than or equal to q. It follows from (5) that $I_\alpha(q)$ and $I_\beta(q)$ are either identical or disjoint. It also follows that any pair of states inside $I_\alpha(q)$ has an overlap $q'\geq q$ and the same is true for $I_\beta(q)$. So we have proven that for any value q_0, by grouping together the states with overlaps $q\geq q_0$, we separate the space of pure states into disjoint clusters. Every cluster is also separated into smaller disjoint clusters when we repeat the same procedure with $q_1>q_0$ and so on. This hierarchical structure of the space of states is characteristic of ultrametric spaces.[13]

We can also compute

$$\overline{P_J(q_1)P_J(q_3)}=\int dq_2\,dq_4\,P(q_1,q_2,q_3,q_4),$$

where $P(q_1,q_2,q_3,q_4)=\overline{P_J(q_1,q_2,q_3,q_4)}$ is the average probability for four states α, β, γ, and δ to have an overlap $q_1=q^{\alpha\beta}$, $q_2=q^{\beta\gamma}$, $q_3=q^{\gamma\delta}$, $q_4=q^{\delta\alpha}$. This computation is very similar to that of $P(q_1,q_2,q_3)$ and we get, after some algebra,

$$\overline{P_J(q_1)P_J(q_2)}$$
$$=\tfrac{1}{3}P(q_1)\delta(q_1-q_2)+\tfrac{2}{3}P(q_1)P(q_2), \quad (7)$$

from which it follows that $\overline{P_J(q_1)P_J(q_2)}\neq P(q_1)P(q_2)$, i.e., $P_J(q)$ is fluctuating even after the thermodynamic limit is taken. We conclude that the order parameter for spin-glasses is the probability distribution of $P_J(q)$ rather than its mean value $P(q)$, i.e., a probability distribution of a probability.

It turns out that this latter probability distribution can, in principle, also be computed. For simplicity, we have calculated the moments μ_r of the probability distribution $\Pi(Y_J(q))$ of $Y_J(q)=\int_q^1 dq'\,P_J(q')$:

$$\mu_r(q)=\int_0^1 dY_J\, Y_J^r\,\Pi(Y_J) \quad (8)$$

for $r=1,\ldots,7$. It can be shown that $\mu_r(q)$ are rth degree polynomials in $y(q)=\overline{Y_J(q)}$ with constant coefficients. This means that $\Pi(Y_J)$ is universal in the following sense: *It depends on all the physical parameters of the system* (the overlap q, the temperature, the magnetic field, etc.) *only through the function $y(q)$, which in turn can be computed in replica scheme by minimizing the free energy of the system.*

As the behavior of $\Pi(Y)$ for $Y\to 1$ is reflected in the large-r behavior of μ_r, we infer that $\Pi(Y)$ has a singularity of the form $(1-Y)^{-y}$. We have reconstructed $\Pi(Y)$ numerically from its moments and the result is shown in Fig. 1. Because of the $(1-Y)^{-y}$ singularity, the most probable value of $Y_J(q)$ [different from its mean value $y(q)$] is 1. The possibility for certain quantities that their most probable value is different from their mean value has been evocated before,[14] but to our knowledge, it is the first time that this is proven in the framework of the replica scheme.

We have also computed the distribution of the clusters into which the space of the spin-glass pure states is divided at any scale q. (In order to take advantage of the universality, we change variables from q to y.) We define the weight W_I of a cluster I (we remind the reader that all the states α which belong to I have a mutual overlap $q^{\alpha\alpha'} \geq q$) by

$$W_I = \sum_{\alpha \in I} P_\alpha.$$

Obviously $\sum_I W_I = \sum_\alpha P_\alpha = 1$.

Let us call $f_J(W,y)\,dW$ the number of clusters having weights between W and $W+dW$. We found that

$$\overline{f_J(W,y)} = \frac{W^{y-2}(1-W)^{-y}}{\Gamma(y)\Gamma(1-y)}. \tag{9}$$

It follows that the average multiplicity of clusters $\int_0^1 dW\, \overline{f_J(W,y)}$ is infinite and this for any value of y. (We remind the reader that $0 \leq y \leq 1$.) This infinite number of clusters is mostly concentrated around $W \simeq 0$. The total weight of these $W \sim 0$ clusters is

$$\int_0^\epsilon dW\, W\overline{f_J(W,y)} \sim \epsilon^y \to 0.$$

So any particular one of them has an extremely small weight.

$y(q)$ has an alternative interpretation: The clusters, at the scale q, have an average weight y:

$$\int_0^1 dW\, W^2\overline{f_J(W,y)} = y = \sum_I W_I^2. \tag{10}$$

Choosing $q = q_{\text{E.A.}}$, in which case it can be shown that each cluster contains only one state, one gets

$$\lim_{q \to q_{\text{E.A.}}} y(q) = \sum_\alpha P_\alpha^2. \tag{11}$$

It is usually believed that the $q(x)$ function has a plateau at $q = q_{\text{E.A.}}$; in this case one has $\sum_\alpha P_\alpha^2$ = length of the plateau. As $P_\alpha < 1$, a few states must dominate this sum.

We shall now briefly discuss the physical implications of our computations. A lot on the nature of the spin-glass phase has been learned from numerical simulations. In order to eliminate large fluctuations and improve the accuracy in a reasonable computer time, the computed quantities have been averaged over the coupling distribution. We have shown that the order parameter is a probability over the coupling distributions. Many numerical simulations will have to be redone in order to compute probability distributions instead of mean values only.

The other striking result we have obtained is the ultrametric topology of the space of pure states. In mathematics, the simplest example of an ultrametric space is shown in Fig. 2 and will be inter-

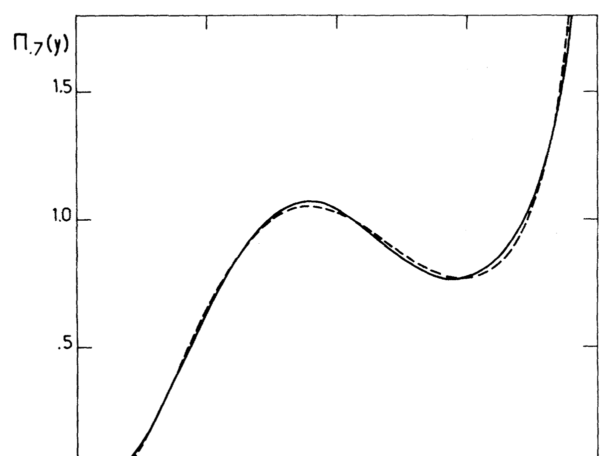

FIG. 1. Probability distribution $\Pi(Y)$ as a function of Y, for the value $y = 0.7$. The dashed curve is the probability obtained by inverting the first six moments μ_r, while the full line is obtained from the first seven moments.

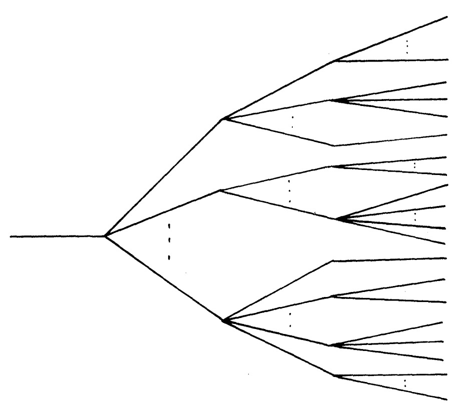

FIG. 2. Hierarchical structure of the ensemble of spin-glass states. The end points represent states; branches (with all their descendents) represent clusters.

preted here as a genealogical tree. The distance between two end points is defined as the number of generations one has to go back in order to find a common ancestor.

The space of pure spin-glass states can be represented with such a picture. End points correspond to states. Branches (with all their descendents) represent clusters. By cutting the tree at any abscissa, one gets a new, shorter genealogical tree. This picture suggests a succession of phase transitions, represented by the branching points. Heating up the system would correspond to cutting the tree at a smaller abscissa: The clusters of low-temperature states become the states of the system at a higher temperature. We found that this number is infinite for any y, i.e., at any temperature, below the spin-glass transition. This means that at least the initial point of the tree has an infinite number of descendents. A similar picture of successive phase transitions has already been proposed.[15] In a recent simulation of a Heisenberg spin-glass at zero temperature, there is some evidence that the states are grouped in discrete clusters.[16]

Finally, we would like to emphasize that all our results have been obtained within the framework of replica symmetry breaking. It would be interesting to obtain the same results by different methods.

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