Order Parameter for Spin-Glasses

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An order parameter for spin-glasses is defined in a clear physical way: It is a function on the interval 0–1 and it is related to the probability distribution of the overlap of the magnetization in different states of the system. It is shown to coincide with the order parameter introduced by use of the broken replica-symmetry approach.

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The mean-field theory for spin-glasses has been obtained in the framework of the replica approach: In the phase where the replica symmetry is spontaneously broken the order parameter is a function $Q(x)$ defined on the interval 0–1.[1] Although a similar order parameter has been obtained in a dynamical approach,[2] the physical meaning of this order parameter is unclear. In this note I define a physically motivated order parameter which I show to be equal to the order parameter of the conventional replica approach.

We consider an Ising spin system, the total number of spins (N) being sufficiently large so that we stay near the thermodynamic limit. As usual, the statistical expectation values are given by

$$\langle O(\sigma)\rangle = \frac{\sum_{\{\sigma\}} O(\sigma)\exp[-\beta H(\sigma)]}{\sum_{\{\sigma\}}\exp[-\beta H(\sigma)]}, \tag{1}$$

$O(\sigma)$ and $H(\sigma)$ being an observable and the Hamiltonian, respectively.

It is well known that in the presence of spontaneous magnetization Eq. (1) must be modified: It predicts zero magnetization at zero magnetic field for all temperatures. Equation (1) does not describe a pure state (thermodynamic phase) of the system but a mixture of different states. We can decompose it as the sum of pure equilibrium states[3]:

$$\langle\cdots\rangle = \sum_{\alpha=1}^{M} P_\alpha\langle\cdots\rangle_\alpha, \quad \sum_{\alpha=1}^{M} P_\alpha = 1. \tag{2}$$

For each of the pure states (labeled by α) the spontaneous magnetization may be different from zero, while the connected correlation function should go to zero at large distances (clustering).

In the normal ferromagnetic Ising model M is always 1, unless the magnetic field is zero and the temperature sufficiently low. In this case we have two pure states of positive and negative magnetization. For spin-glasses the situation is quite different: There is good evidence that (especially for the infinite-range model) even for a nonzero magnetic field there are many equilibrium states; the space of configurations consists of many valleys separated by high mountains (free-energy barriers) whose height goes to infinity in the infinite-volume limit.[4] Explicit Monte Carlo simulations have shown that in the infinite-range model the system will not change valleys for a time proportional to $\exp(N^{1/4})$.[5] The total number of valleys seems to increase like a power of N, and so they do not contribute to the zero-temperature entropy. If there is not a one to one correspondence between the pure states of the system at two different values of the magnetic field, hysteresis effects are expected: By changing the magnetic field the system will go to an excited metastable state and decay to the true equilibrium state only after a very large time.[6] In the same way the linear-response susceptibility, which according to Fischer[7] is given by

$$\chi_{\mathrm{LR}} = \beta\Big(1 - \sum_{i=1}^{N}\langle\sigma_i\rangle_\alpha^2/N\Big), \tag{3}$$

is different from the total susceptibility

$$\chi = \beta\Big(1 - \sum_{i=1}^{N}\langle\sigma_i\rangle^2/N\Big), \tag{4}$$

for which the contribution of jumping from one state to another is included.

The existence of many states according to the previous analysis is the main characteristic of the glassy phase and we would like to retain this information in the order parameter.

We first notice that we can characterize the state by the value of the magnetization in each site:

$$m_i^{\alpha} = \langle\sigma_i\rangle_\alpha. \tag{5}$$

For each state we can construct the equivalent

of the Edwards-Anderson order parameter[8]:

$$q_{EA}{}^{\alpha} = \sum_{i=1}^{N} \langle \sigma_i \rangle_{\alpha}{}^2 / N. \tag{6}$$

It is quite reasonable that in the infinite-volume limit all states will have the same value of $q_{EA}{}^{\alpha}$: Equation (6) defines an order parameter which does not make reference to a particular pure state. The serious disadvantage of q_{EA} is that it is different from zero also for a normal unfrustrated ferromagnetic or antiferromagnetic material, not only for a spin-glass.

Something more interesting can be obtained by studying the overlap of the magnetizations between two different states:

$$q_{\alpha\beta} = \sum_{i=1}^{N} m_i{}^{\alpha} m_i{}^{\beta} / N, \qquad P(q) = \textstyle\sum_{\alpha,\beta} P_\alpha P_\beta \delta(q - q_{\alpha\beta}), \tag{7}$$

where $P(q)$ is the probability distribution of the $q_{\alpha\beta}$. We can introduce the function $x(q)$, where

$$x(q) = \int_{-\infty}^{q} dq\, P(q), \tag{8}$$

which is monotonic and an inverse function, which is obviously defined in the interval 0–1.

If the function $q(x)$ is constant, we have only pure states which do not differ macroscopically. If the function $q(x)$ is not a constant, macroscopically different pure states must exist; $q(1)$ is identified with the Edwards-Anderson order parameter, while $q(0)$ is the minimum overlap between two states. The linear-response susceptibility (the reversible one) and the true susceptibility (which should be presumably identified with the field-cooled one) are given by

$$\chi_{LR} = \beta[1 - q(1)], \quad \chi = \beta\left[1 - \int_0^1 q(x)dx\right]. \tag{9}$$

We can thus characterize the glassy phase by a nontrivial dependence of $q(x)$ on x.[9]

Having defined an order parameter having a clear physical meaning, we can now show that this order parameter coincides with the one introduced in the replica approach.[10] The explicit decomposition of a state into its pure components is not a simple operation; a fast way to obtain the function $q(x)$ consists in considering two real replicas of the same system[11] ($\sigma_i{}^a$; $i = 1, N$; $a = 1, 2$) with the Hamiltonian

$$H_2 = \sum_{a=1}^{2} H(\sigma^a). \tag{10}$$

In the infinite-volume limit we have that

$$\langle \exp\Big(y \sum_{i=1}^{N} \sigma_i{}^1 \sigma_i{}^2 / N\Big) \rangle_2 \equiv g(y) \cong \sum_{\alpha=1}^{M} \sum_{\beta=1}^{M} P_\alpha P_\beta \exp(y q_{\alpha\beta}) = \int_0^1 dx\, \exp[y q(x)], \tag{11}$$

where by $\langle \cdots \rangle_2$ we denote the statistical expectation value with the Hamiltonian H_2.[12] Equation (11) is rather interesting. It gives us the possibility of computing $q(x)$ using conventional techniques, like the Monte Carlo method.

In the replica approach one introduces an n times replicated Hamiltonian and the order parameter is an $n \times n$ matrix, which is zero on the diagonal, defined as follows[1]:

$$Q_{ab} = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i{}^a \sigma_i{}^b \rangle, \quad a \neq b, \quad Q_{aa} = 0. \tag{12}$$

In the presence of symmetry breaking in replica space the matrix Q_{ab} has a nontrivial dependence on the indices. The naive expression for $g(y)$,

$$g(y) = \exp(y Q_{12}), \tag{13}$$

must be modified[13] by summing over all the possible ways in which the symmetry may be broken in replica space. We finally obtain

$$g(y) = \frac{1}{n(n-1)} \sum_{\substack{a=1 \\ a \neq b}}^{n} \sum_{b=1}^{n} \exp(y Q_{ab}). \tag{14}$$

In the approach of Ref. 1 the matrix Q_{ab} was characterized by a function $Q(x)$ defined on the interval 0–1; if we go back to the original definitions, we easily find that for $n \to 0$

$$g(y) = \int_0^1 dx \exp[y Q(x)]. \tag{15}$$

The functions $Q(x)$ and $q(x)$ are therefore identified, the physical interpretation of $Q(x)$ now being clear.

We notice, *en passant*, that a rather simple expression for $q(0)$ can be obtained if we consider the function $q(h_1, h_2)$ defined as

$$q(h_1, h_2) = \frac{1}{N} \sum_{i=1}^{N} m_i(h_1) m_i(h_2). \tag{16}$$

Similar arguments, which will be reported in detail elsewhere,[14] tell us that[9]

$$\lim_{h_2 \to h_1} q(h_1, h_2) = q(0) \neq q(h_1, h_1) = \int_0^1 dx\, q(x). \tag{17}$$

In other words $q(0)$ is the average overlap between two states[15] at different but similar magnetic fields.

It is now clear that the mysterious breaking of the replica symmetry is just the mathematical transcription of the existence of infinitely many pure thermodynamic states.

The definition of the order parameter $q(x)$ does not make reference to the fact that for spin-glasses the Hamiltonian H is random. It is unclear to me if other amorphous materials (like real glasses or hard spheres at high density) have many different pure states when the volume goes to infinity so that the definition of the order parameter presented here can be successfully extended.

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[9]By comparing Eqs. (2), (4), and (7), it follows that

$$\frac{1}{N}\sum_{1}^{N}\langle\sigma_i\rangle^2 = \frac{1}{N}\sum_{\alpha,\beta}\sum_{1}^{N} P_\alpha P_\beta m_i^\alpha m_i^\beta = \int dq\, qP(q) = \int_0^1 dx\, q(x).$$

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