Direct Determination of the Probability Distribution for the Spin-Glass Order Parameter

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The recent interpretation of Parisi's order-parameter function $q(x)$ in terms of a probability distribution for the overlap between magnetizations in different phases is investigated by Monte Carlo computer simulation for the infinite-range Ising spin-glass model. The main features of the solution for $q(x)$ are reproduced, in particular $q(x) \propto x$ as $x \to 0$ and $q'(x) = 0$ at $q = q_{\max}$, the largest value. Finite-size effects prevent one from establishing with certainty whether there is a "plateau," i.e., $q'(x) = 0$ for a range of x.

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The replica technique used to be a great mystery when applied in situations[1] where it was necessary to "break replica symmetry." It has been applied particularly to the infinite-range Ising spin-glass model of Sherrington and Kirkpatrick[2] (SK) and the most interesting results have been obtained by Parisi.[3] In his theory replica-symmetry breaking shows up as an order-parameter function $q(x)$ for $0 \le x \le 1$. Recently, however, the replica technique has become much better understood following the observation[4] that statistical-mechanics expectation values are obtained by integrals over x; e.g.,

$$q = \langle\langle S_i\rangle_T^2\rangle_J = \int_0^1 q(x)dx$$
$$q^{(2)} = \langle\langle S_iS_j\rangle_T^2\rangle_J = \int_0^1 q^2(x)dx \quad (i \ne j), \tag{1}$$

where $S_i = \pm 1$ is an Ising spin, $i = 1, \ldots, N$, $\langle \ldots \rangle_T$ denotes a statistical-mechanics average for a given set of interactions, and $\langle \ldots \rangle_J$ is an average over interactions. Subsequently it was shown[5] that one can interpret not just integrals over x but $q(x)$ for any particular value of x. The main ingredient in the argument is that the SK model can exist in one of many phases, which are stable for $N \to \infty$. If one defines the magnetization of site i when the system is in phase s by m_i^s and $q^{ss'}$, the overlap between magnetizations, by

$$q^{ss'} = \frac{1}{N}\sum_{i=1}^N m_i^s m_i^{s'}, \tag{2}$$

then the derivative of the inverse function, i.e., dx/dg, turns out to be a probability distribution for overlap between magnetizations of solutions, i.e.,

$$\frac{dx}{dq} = W(q) = \langle \sum_{s,s'} P(s)P(s')\delta(q^{ss'} - q)\rangle_J, \tag{3}$$

where $P(s)$ is the Boltzmann weight[4] associated with solution s. In particular, changing the integration variable in Eq. (1) from x to q, one finds that q and $q^{(2)}$ are just the first two moments of the distribution $W(q)$, namely,

$$q = \int q'W(q')dq', \quad q^{(2)} = \int q'^2W(q')dq'. \tag{4}$$

Recently,[6] both q and $q^{(2)}$ have been calculated by computer simulations at a fixed temperature below the transition temperature T_c for several sizes and the results appear to extrapolate to Parisi's values for $N \to \infty$. However, a much more dramatic test of the theory would be to reproduce the entire distribution $W(q)$. This Letter describes numerical simulations of $W(q)$ for several finite sizes which do indeed reproduce many of the features of Parisi's function $q(x)$. Before giving the numerical data it is necessary to describe what Parisi's equations give for $W(q)$.

Rather than plot $q(x)$ against x, as is conventional, I sketch in Fig. 1 the inverse function $x(q)$, since $W(q)$ is just the derivative of this. Above the de Almeida–Thouless[7] (AT) line there is only one phase, the SK solution is correct, and $x(q)$ is a unit step function at $q = q_{\rm SK}$, the SK value, so that

$$W(q) = \delta(q - q_{\rm SK}). \tag{5}$$

For $h \to 0$, on the other hand, Parisi's theory predicts[3,8] that $x(q)$ has a smooth part, starting at the origin and ending at $x = \bar{x}$, $q = q_{\max}$, at which point there is step to $x = 1$, so that

$$W(q) = \overline{W}(q) + (1 - \bar{x})\delta(q - q_{\max}), \tag{6}$$

where $\overline{W}(q)$ is the smooth part of the distribution and has weight $\bar{x}$. Since $x \propto q$ as $q \to 0$, then $\overline{W}(q)$ is finite as $q \to 0$. Obviously $\overline{W}(q)$ is zero for $q > q_{\max}$.

Next I discuss the numerical simulations. The Hamiltonian is given by

$$H = -\sum_{\langle i,j\rangle} J_{ij}S_iS_j - h\sum_i S_i, \tag{7}$$

where the J_{ij} are Gaussian random variables with zero mean and variance[2,9] $J/(N-1)$, and h is a uniform field. For $N \to \infty$ there is a transition in

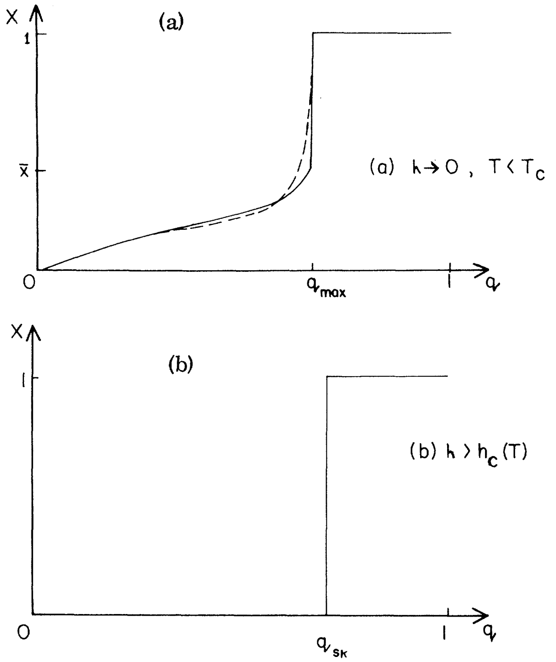

FIG. 1. The solid lines are sketches of the function $x(q)$ from Parisi's theory. In (a), the dashed curve is similar to Parisi's results but with the vertical piece rounded out. The numerical simulations on moderate sizes cannot distinguish between these possibilities. In (b), $h_c(T)$ is the critical de Almeida–Thouless field and q_{SK} is the SK value for the spin-glass order parameter.

zero field at $T_c = J$. It is useful to simulate at the same time two independent samples with the *same* interactions and field. These two samples are simulated up to a time t_0, to equilibrate, before any averaging is done. It is necessary that t_0 is longer than the longest relaxation time,[10] τ, which diverges when $N\to\infty$. However, previous work[11] has obtained the relaxation times at $T = 0.4T_c$, $h = 0$, and so we shall concentrate on this point in the h-T plane and make sure that t_0 is large enough for each size.

For $t > t_0$ one then calculates

$$Q(t) = \frac{1}{N}\sum_{i=1}^{N} S_i^{\,1}(t_0+t) S_i^{\,2}(t_0+t), \tag{8}$$

where the superscripts 1 and 2 on S_i refer to the two identical samples. The distribution of $Q(t)$ is independent of t and is obtained from

$$W(q) = \left\langle \frac{1}{T}\sum_{t=1}^{T} \delta(q - Q(t)) \right\rangle_J. \tag{9}$$

With use of an integral representation of the delta function it is straightforward to show that for $N\to\infty$ the distribution is the same as that in Eq. (3). Furthermore, standard statistical arguments predict that if the system exists in just a single phase then, for a large finite system, $W(q)$ is a Gaussian distribution of width of order $N^{-1/2}$, which of course goes over to the delta function of Eq. (5) in the thermodynamic limit.

Above the AT line I find precisely this Gaussian behavior, showing that there is only one phase available to the system. By contrast the results for $W(|q|)$ at $h = 0$, $T = 0.4T_c$, shown in Fig. 2, have a peak at large $|q|$ but also a long tail extending to $|q| = 0$ with a finite weight there. Since the model has time-reversal symmetry $W(q)$ is symmetric[12] and so I plot the distribution against $|q|$. Consider first of all the small-q region in more detail. All sizes show a finite value for $W(0)$ with no sign of this vanishing for $N\to\infty$. In fact, there is some suggestion of an upturn in the curve as $|q|\to 0$ for larger sizes though this is not really outside the statistical errors. Interestingly, it appears that the solution of Parisi's theory does have such an upturn.[8] Since a direct solution of Parisi's equations is very complicated, in order to compare the numerical data with the theory I have used the scaling *Ansatz* of Ref. 8 that $q(x,T) = F(x/T)$ for $x \le \bar{x}$ to determine $q(x)$. The only extra information needed is $q_{max}(T)$. I use the approximate formula

$$q_{max}(T) = 1 - 2\left(\frac{T}{T_c}\right)^2 + \left(\frac{T}{T_c}\right)^3, \tag{10}$$

which correctly gives the first three terms in the expansion[13] about $T = T_c$ and correctly gives a T^2 dependence at low temperatures. The resulting prediction for $W(q)$ is shown by the dotted line in Fig. 2. The upturn at low q is more pronounced than in the numerical results.

Next let us look at the region of the peak in $W(q)$. The peak position shifts to smaller q values as N increases, consistent with the value 0.744, from Eq. (10), for $N\to\infty$, although reliable extrapolation is not possible because of uncertainties in the data and because the form of the leading size correction is not known. The peak also becomes narrower as N increases, particularly on the high-q side, indicating that $W(q)$ is strictly zero for q bigger than some q_{max} when $N\to\infty$. However, on the low-q side of the peak the results appear to differ more and more from the approximate analytic solution of Parisi's equations (shown by the dotted line) as N increases. This could indicate that $\overline{W}(q)$ diverges as $q \to q_{max}$, or in other words, $dq/dx \to 0$ as $q\to q_{max}$. Such a possibility would occur, for instance, if

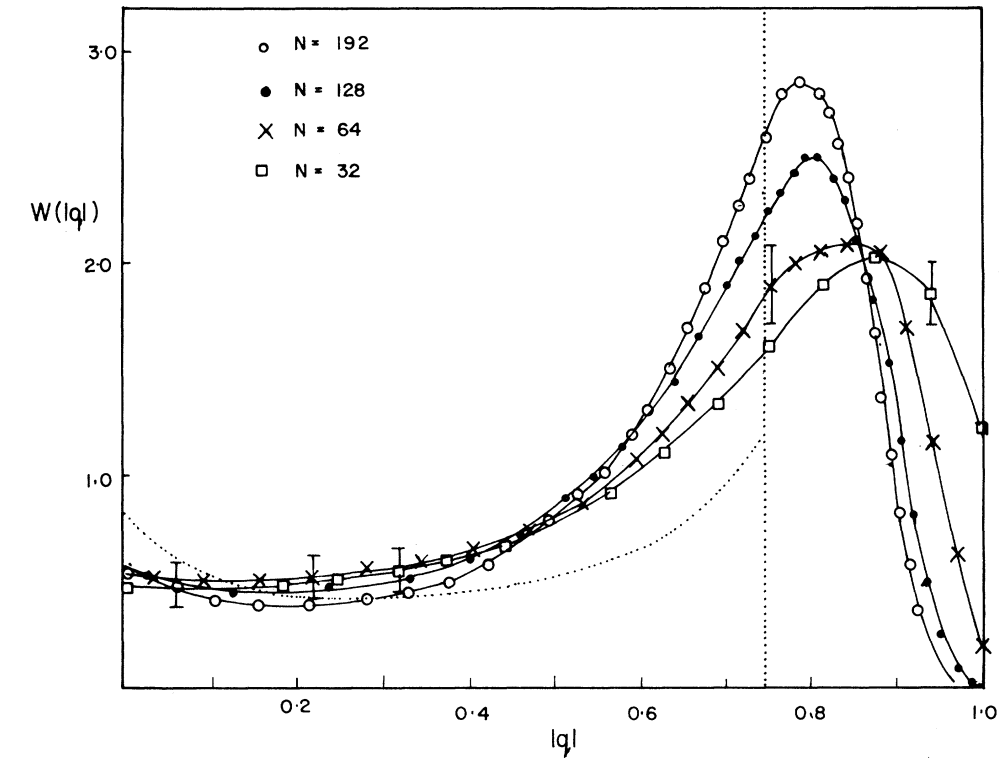

FIG. 2. $W(|q|)$ for $T = 0.4T_c$, $h = 0$. Some typical error bars are shown. The data clearly indicate a tail in $W(|q|)$ extending down to $q = 0$, which corresponds to the existence of many phases some of which have zero overlap between their magnetizations. There is also clear evidence that for $N \to \infty$ a divergence in $W(|q|)$ occurs at a maximum value, $q_{\max}$, beyond which $W(q)$ is zero. The dotted line is obtained from a scaling Ansatz for Parisi's equations, as described in the text. There is a delta function of weight $\frac{4}{7}$ at $q = q_{\max} = 0.744$ and a continuous part which has a pronounced upturn as $q \to 0$.

dq/dx is only zero at $x = 1$, i.e., the "plateau" in $q(x)$ is rounded out, as shown by the dashed line in Fig. 1(a). Another possibility is that a plateau region in $q(x)$ does occur but that the rest of the curve joins the plateau region with zero slope. It should be pointed out, though, that the *position* of the peak is also shifting with increasing N and this may account for the data for larger sizes deviating more from the dotted line in Fig. 2. It is possible that for much larger sizes, where the shift in the peak becomes negligible, one would see the numerical results approaching the analytic theory. One cannot really distinguish between these various possibilities from the available data.

To conclude, I have shown that many features of Parisi's order-parameter function are reproduced by the simulations, in particular, $q(x) \propto x$ as $x \to 0$ and $q'(x) = 0$ at $q = q_{\max}$. Parisi's theory is therefore at least an excellent approximation to the solution of the SK model and may well be the exact solution. It would help comparison with numerical data if accurate solutions for the functions $q(x)$ were available. The computations also provide strong support for the arguments of Ref. 4 that statistical-mechanics averages are obtained from integrals over x (which differs from Sompolinsky's[14] dynamical interpretation) and for the subsequent interpretation[5] of dx/dq as a probability distribution for overlap between magnetizations of phases. This insight into the physical significance of replica-symmetry breaking may be useful in other situations, for instance a ferromagnet with finite-range interactions in a random field[15] which is of considerable interest at the moment.

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[1]See, e.g., A. J. Bray and M. A. Moore, Phys. Rev. Lett. 41, 1068 (1978); G. Parisi, Phys. Rev. Lett. 43,

1574 (1979), and J. Phys. A 13, L115, 1101, 1887 (1098), and Philos. Mag. 41, 677 (1980).

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[3]Parisi, Ref. 1.

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[6]N. D. Mackenzie and A. P. Young, to be published.

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[8]J. Vannimenus, G. Toulouse, and G. Parisi, J. Phys. (Paris) 42, 565 (1981).

[9]A. P. Young and S. Kirkpatrick, Phys. Rev. B 25, 440 (1982).

[10]For $h=0$ there is an additional longer time, τ_{eg}, which corresponds to "turning over" all the spins; see N. D. Mackenzie and A. P. Young, Phys. Rev. Lett. 49, 301 (1982). However, we know that all these fluctuations do is symmetrize $W(q)$, so that I simply run the simulation for time τ and then symmetrize $W(q)$ by hand.

[11]Mackenzie and Young, Ref. 10.

[12]Note that Parisi's solution also gives a symmetric $W(q)$ in strictly zero field because one should average over all equivalent saddle points, including those generated by time-reversal symmetry; see Ref. 4.

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[15]A. J. Bray and M. A. Moore, unpublished; G. Parisi, unpublished.