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1983 J. Phys. A: Math. Gen. 16 L199

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J. Phys. A: Math. Gen. **16** (1983) L199–L204. Printed in Great Britain

LETTER TO THE EDITOR

Spontaneous symmetry breaking in spin glasses

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Received 2 February 1983

Abstract. We discuss the effect of a small uniform symmetry breaking field on the Sherrington–Kirkpatrick spin glass model. Both $q(h)=\langle\langle S_i\rangle_T^2\rangle_J$ and $q_{ij}(h)=N\langle\langle S_i\rangle_T\langle S_j\rangle_T-\langle S_iS_j\rangle_T\rangle_J$ are given by scaling functions, $f(h/h^*)$ and $g(h/h^*)$ respectively, where $h^*=T/N^{1/2}$. We show that $g(x)=xf'(x)$ so that in the symmetry broken situation ($h/h^*\to\infty$ but $h\ll 1$) we have $f(x)\to q$, the statistical mechanics order parameter, and $g(x)\to q_{ij}=0$. The latter is in contrast to the conclusions of Young and Kirkpatrick based on numerical evidence for small samples. We discuss the reasons for this discrepancy.

It is by now rather well established (Young and Kirkpatrick 1982, to be referred to as YK, Sompolinsky 1981, Young 1981, de Dominicis and Young 1983, Mackenzie and Young 1982, Toulouse 1982, Hertz 1982) that the Sherrington–Kirkpatrick (1975) model exhibits non-ergodic behaviour. One result is that many order parameters can be defined. Here we confine our attention to statistical mechanics averages, and the corresponding order parameter

$$q=\lim_{h\to 0}\lim_{N\to\infty} q_N(h) \tag{1}$$

with

$$q_N(h)=\langle\langle S_i\rangle_T^2\rangle_J$$

where h is the field, $S_i=\pm 1$ denotes the ith ($i=1\ldots N$) Ising spin, $\langle\ldots\rangle_T$ denotes a statistical mechanics average for a given set of interactions J_{ij} and $\langle\ldots\rangle_J$ indicates an average over the J_{ij}. We assume a symmetric distribution for the J_{ij} of width N^{-1} so the transition occurs at temperature $T_c=1$ (with Boltzmann's constant set equal to unity). The order of limits in (1) is important because for each size N there is a critical field h^* (which vanishes as $N\to\infty$) such that for $h\ll h^*$ the thermal average gives zero because of time reversal symmetry, while for $h\gg h^*$ the symmetry is broken and we have the possibility of a non-zero value. It has earlier been argued (YK) that

$$h^*=T/N^{1/2} \tag{2}$$

because the magnetisation of low energy states is of order $N^{1/2}$. We shall consider only a uniform field, but (2) also applies (YK) to a completely random staggered field $\pm h$. We shall not consider the possibility of complicated staggered fields conjugate to one of the minima in phase space (and which therefore depend on the J_{ij}) for which possibly $h^*\sim N^{-1}$. We shall consider a large but finite system and investigate the regions $h>h^*$ and $h<h^*$ but always with $h\ll 1$. The symmetry breaking situation

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in (1) therefore corresponds to

$$h/h^* \to \infty, \qquad h \ll 1. \tag{3}$$

The only dependence of $q_N(h)$ on N will be through the N dependence of h^*, so we shall not indicate the N dependence explicitly from now on.

Another quantity of interest is the uniform susceptibility $\chi(h)$, which is related to $q(h)$ by the fluctuation–dissipation theorem:

$$T\chi(h) = N^{-1} \sum_{i,j} \langle\langle S_iS_j\rangle_T - \langle S_i\rangle_T\langle S_j\rangle_T\rangle_J = 1 - q(h) - q_{ij}(h) \tag{4}$$

where

$$q_{ij}(h) = N\langle\langle S_i\rangle_T\langle S_j\rangle_T - \langle S_iS_j\rangle_T\rangle_J \qquad (i \neq j) \tag{5}$$

is the contribution from the off-diagonal terms. For a symmetric distribution of J_{ij} and h *strictly* zero q_{ij} vanishes (e.g. Fischer 1976). However, YK pointed out that h strictly zero is different from the limits in (3) and argued on the basis of numerical results that q_{ij} is finite in the symmetry broken situation below T_c.

In this paper we investigate in more detail the behaviour of $q(h)$ and $q_{ij}(h)$ for $h \sim h^*$ by a series expansion in powers of h/h^*. If we define

$$q(h) = f(h/h^*), \qquad q_{ij}(h) = g(h/h^*), \tag{6}$$

then

$$q = \lim_{x\to\infty} f(x) \tag{7a}$$

and, defining q_{ij} in a similar way,

$$q_{ij} = \lim_{x\to\infty} g(x), \tag{7b}$$

then the claim of YK is that $q_{ij} \neq 0$ below T_c. However, we show below that

$$g(x) = xf'(x) \tag{8}$$

and since $f(x) \to$ constant as $x \to \infty$ it follows that $q_{ij} = 0$. Later on we discuss why the conclusion of YK turns out to be incorrect. We also relate our results to the claim of Sompolinsky (1981) that q also vanishes.

To proceed we note that $1 - q(h) = \langle\langle S_iS_i\rangle_c\rangle_J$, where $\langle\ \rangle_c$ denotes a cumulant (statistical mechanics) average. The uniform field couples to the total magnetisation M $(= \Sigma_{j=1}^N S_j)$. Hence if we expand $1 - q(h)$ as a series in powers of h then u_n, the coefficient of h^n, is given by

$$u_n = (1/n!)\langle\langle S_iS_i(M/T)^n\rangle_c\rangle_J$$

where the averages are for h strictly zero. Noting that coefficients of odd powers of h vanish we define

$$f(x) = \sum_{n=1}^{\infty} a_n x^{2n} \tag{9}$$

and obtain

$$a_n = [-1/(2n)!](h^*/T)^{2n}\langle\langle S_iS_iM^{2n}\rangle_c\rangle_J. \tag{10}$$

Next we pick out the dominant contribution to (10), i.e. those terms with the largest number of independent summations over sites. Since each site must occur an even number of times for the average to be non-zero, we divide the $2n$ spins from the factor M^{2n} into n pairs such that the spins of each pair refer to the same site. The summations give a factor of N^n, so one finds

$$a_{2n} = (-1/2^n n!)\langle\langle S_1S_1S_2S_2 \ldots S_{n+1}S_{n+1}\rangle_c\rangle_J \tag{11}$$

where we have used (2).

The calculation of $g(x)$ proceeds in a similar way. Defining

$$g(x) = \sum_{n=1}^{\infty} b_n x^{2n} \tag{12}$$

one finds

$$b_n = [-N/(2n)!](h^*/T)^{2n}\langle\langle S_iS_jM^{2n}\rangle_c\rangle_J$$

where $i \neq j$. In order to pair up the sites one of the $2n$ spins from the factor M^{2n} has to be site i, another site j and the remaining $2n-2$ divided into $(n-1)$ pairs. Consequently we obtain

$$b_n = [-1/2^{n-1}(n-1)!]\langle\langle S_1S_1S_2S_2 \ldots S_{n+1}S_{n+1}\rangle_c\rangle_J = 2na_n \tag{13}$$

so that

$$g(x) = xf'(x) \tag{8}$$

which implies $q_{ij} = 0$ as discussed above.

It is useful to evaluate explicitly the first term

$$b_1 = -(\langle\langle S_1S_1S_2S_2\rangle_T - \langle S_1S_1\rangle_T\langle S_2S_2\rangle_T - 2\langle S_1S_2\rangle_T^2\rangle_J) = 2\langle\langle S_1S_2\rangle_T^2\rangle_J. \tag{14}$$

Defining

$$q^{(2)} = \langle\langle S_1S_2\rangle_T^2\rangle_J \tag{15}$$

then

$$q^{(2)} = 1 - 2T|U(T)| \tag{16}$$

(Bray and Moore 1980) where $U(T)$ is the energy per spin. $q^{(2)}$ is therefore certainly non-zero below T_c because there is compelling numerical evidence (Kirkpatrick and Sherrington 1978, Mackenzie and Young 1983) that $U(T)$ deviates from its paramagnetic value of $-1/2T$ below T_c. We shall return to this point later on. It follows from (14) that $b_1 \neq 0$, as was noted by YK. Hence $g(x) \to 0$ both for $x \to 0$ and $x \to \infty$ but is finite for intermediate values of x. This non-monotonic behaviour was not anticipated by YK.

Higher-order terms in the expansions involve more complicated correlation functions. For instance, the coefficient of h^4 is proportional to $q^{(3)} = \langle\langle S_1S_2\rangle_T\langle S_2S_3\rangle_T\langle S_3S_1\rangle_T\rangle_J$. Below T_c replica symmetry is broken (see e.g. Parisi 1980 and references therein) and there is no simple relationship between the 'order parameters' which appear in successive terms. However, we can obtain closed form expressions for f and g if we make a single order parameter ansatz, that is to say all order parameters are assumed to be powers of q, e.g. $q^{(2)} = q^2$, $q^{(3)} = q^3$. In this case one has

$$\langle\langle S_1S_1S_2S_2 \ldots S_{n+1}S_{n+1}\rangle_c\rangle_J = c_n q^{n+1} \tag{17}$$

where c_n is a numerical factor. Hence from (6), (9), (11) and (17) one obtains

$$q(h) = q\bar{f}(q^{1/2}h/h^*) \tag{18}$$

with

$$\bar{f}(x) = -\sum_{n=1}^{\infty} \frac{c_n}{2^n n!} x^{2n}. \tag{19}$$

Clearly for consistency we must have $\lim_{x\to\infty} \bar{f}(x) = 1$. We shall now obtain $\bar{f}(x)$ explicitly and verify this. The factor of c_n in (17) comes from expanding out the cumulant average, setting to zero an average of a product of an odd number of spins and setting to unity an average of an even product of spins. Hence c_n is just the $2n$th cumulant average of a single free spin, i.e.

$$c_n = \langle S^{2n} \rangle_c. \tag{20}$$

Let us therefore consider a set of free spins in fields h_i and repeat the above calculation for $\langle\langle SS\rangle_c\rangle_h = 1 - \bar{q}(h)$ where $\langle \ldots \rangle_h$ is an average over the distribution of the h_i. One readily finds (incorporating temperature into h)

$$\bar{q}(h) = -\sum_{n=1} \frac{\langle S^{2n}\rangle_c}{(2n)!} \langle h^{2n} \rangle_h \tag{21}$$

where $\langle \ldots \rangle_c$ is for a single spin in zero field as in (20). Hence if we choose a Gaussian distribution for the h_i, so that $\langle h^{2n}\rangle_h = x^{2n}(2n)!/(2^n n!)$ where x is the standard deviation, one obtains $\bar{q}(h) = \bar{f}(x)$. But $\bar{q}(h)$ is trivial for this single-site problem. Thus

$$\bar{f}(x) = (2\pi x)^{-1/2} \int_{-\infty}^{\infty} \exp(-y^2/2x) \tanh^2 y \, \mathrm{d}y. \tag{22}$$

Similarly for $q_{ij}(h)$ we obtain with a single order parameter ansatz

$$q_{ij}(h) = q\bar{g}(q^{1/2}h/h^*)$$

where

$$\bar{g}(x) = x\bar{f}'(x). \tag{23}$$

The functions $\bar{f}(x)$ and $\bar{g}(x)$ are plotted in figure 1. Notice that the sum $\bar{f} + \bar{g}$ (which determines $\chi(h)$ and hence the magnetisation, see (4)) approaches its asymptotic value faster than $\bar{f}$ or $\bar{g}$ separately because the leading correction ($\sim 1/x$) cancels in the sum.

Next we discuss why YK incorrectly concluded that $q_{ij} \neq 0$. YK calculated χ and q and noted that $T\chi \neq 1 - q$, the discrepancy increasing as N increased. The difference must be made up by q_{ij}, see (4), which was therefore argued to be non-zero. However, YK did not evaluate q directly by applying a field and taking the limits in (3) because these limits cannot be simultaneously satisfied for a small system. Instead, YK argued that the effect of the uniform field could be represented by projecting out states with a positive magnetisation. Let us denote an average over this restricted ensemble by $\langle \ldots \rangle'_T$. It is instructive to consider the effect of a magnetic field on these restricted averages and we denote the corresponding value of $\langle\langle S_i\rangle_T'^2\rangle_J$ by $q'_N(h)$ (NB the prime does not indicate a derivative). YK assumed that the order of the limits $h \to 0$ and $N \to \infty$ can be interchanged in $q'_N(h)$, i.e. if

$$q' = \lim_{N\to\infty} q'_N(h=0)$$

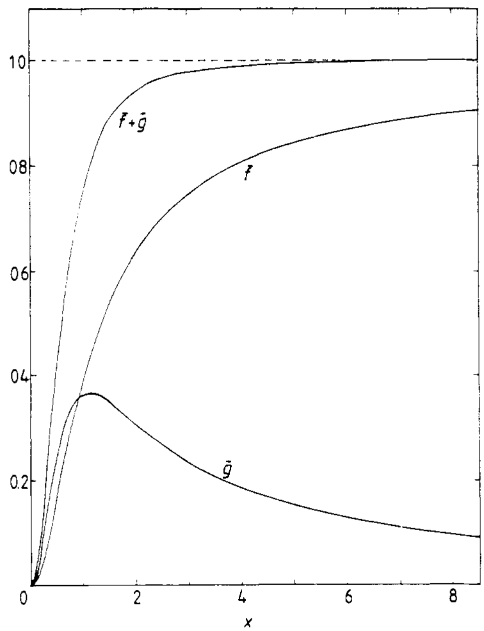

Figure 1. The function $\bar{f}(x)$ is given by (22) and $\bar{g}(x)$ is related to $\bar{f}(x)$ by $\bar{g}(x) = x\bar{f}'(x)$. The sum of the two functions is also plotted and is seen to approach its asymptotic value (of 1) faster than $\bar{f}(x)$ or $\bar{g}(x)$ separately approach their asymptotic values (of 1 and 0 respectively).

then according to YK

$$q = q'. \tag{24}$$

In view of our above calculation the assumption that the order of limits can be interchanged must be incorrect. We suggest that for a large system $q(h)$ and $q'(h)$ vary as shown in figure 2. YK calculated q' for several small sizes and interpreted it as q whereas, in fact, all we can say is that

$$q > q', \tag{25}$$

assuming that $q'(h)$ is an increasing function of h which seems likely. If q is larger than that claimed by YK then the relation $T\chi = 1 - q$ can be satisfied and hence $q_{ij} = 0$. YK also noted that their results for q seemed to be incompatible with Parisi's (1980) theory, but in view of the above discussion YK values for q are inaccurate, so this discrepancy is removed.

Finally, we situate our results in the context of Sompolinsky's (1981) prediction that $q = 0$. One way that q could be zero would be if all coefficients in the expansion were zero, which implies a zero value $q^{(2)}$, $q^{(3)}$ etc (i.e. order parameters which are not required to be zero *by symmetry* in strictly zero field). However, as noted above $q^{(2)}$ is related to the energy by (16) and so we are certain that $q^{(2)} > 0$ at low temperatures. Hence all coefficients cannot vanish. On the other hand, it seems unlikely that q could vanish at all temperatures if the coefficients in the expansion are finite. Our results are, however, quite consistent with the argument of de Dominicis and Young (1983) that, within the replica formalism, statistical mechanics expectation

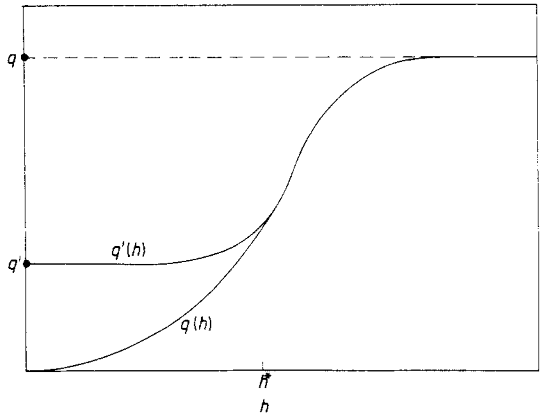

Figure 2. A sketch of the expected variation of $q(h)$ and $q(h')$ for a large sample. The position of h^*, defined by (2), is shown. q is defined by the value of $q(h)$ in the limit $h/h^* \to \infty$ (but $h \ll 1$). q' is defined by $q'(h=0)$ and clearly $q' < q$. The quantity calculated by YK was actually q' rather than q.

values are obtained by averaging over all replicas. Within the Parisi (1980) scheme this gives $q = \int_0^1 q(x)\,\mathrm{d}x$, $q^{(2)} = \int_0^1 q^2(x)\,\mathrm{d}x$ etc. For these replica averaged quantities and to lowest order in t $(=1-T)$ Parisi finds that a single order parameter description holds, with $q^{(2)} = q^2$ etc and $q = t$. This just corresponds to our equation (18) with $q = t$.

Furthermore we have argued (equation (25)) that q' provides a lower bound for q and the data of YK indicate clearly that $q' > 0$. Additional results on larger samples using Monte Carlo simulation (Mackenzie and Young 1983) confirm this prediction.

To conclude, we have shown that $q_{ij} = 0$, so $T\chi = 1 - q$, as $h \to 0$. There are consequently no numerical results, to our knowledge, which conflict with Parisi's theory (if the latter is correctly interpreted).

One of us (SJ) would like to thank the SERC for a research studentship.

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