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LETTER TO THE EDITOR

Series expansions for a spin-glass model

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Abstract. Series expansions are investigated for a spin-glass Ising model with nearest-neighbour interactions J which can be randomly positive or negative. For the high-temperature phase the following conclusions result:—(i) the free energy has a singularity at about $w = \mu^{-1/2}$ ($w = \tanh \beta J$) (where μ is the self-avoiding walk limit), (ii) the magnetic susceptibility corresponds to uncoupled spins, (iii) the second derivative of susceptibility is simply related to the susceptibility of the standard Ising model and has a singularity at $w = w_c^{1/2}$ (where w_c refers to the standard model). Higher derivatives can be dealt with similarly. The low-temperature phase is more difficult to deal with because of the degeneracy of the lowest energy state. Further investigation is needed to decide whether the experimentally observed singularities correspond to the above, or arise as discontinuities from the meeting of the two phases.

The behaviour of spin-glasses with randomly competing ferromagnetic and antiferromagnetic interactions, but no long-range magnetic order, has given rise to a number of theoretical investigations recently. Adkins and Rivier (1974) suggested that the experimentally observed cusp in magnetic susceptibility should be associated with the disappearance of short-range order. Edwards and Anderson (1975) constructed an alternative theory based on the concept of particular 'glassy' ground states, any of which would 'disorder' with increasing temperature, ultimately giving rise to a singularity which is a cusp in magnetic susceptibility. Both of the above treatments made use of an approximation of mean-field type.

Sherrington and Kirkpatrick (1975) put forward a model of a spin-glass with long-range interactions for which they were able to derive an exact solution. Considering a Gaussian distribution of interactions with mean J_0 and standard deviation ΔJ, they obtained results analogous to those of Edwards and Anderson for a certain range of the parameter $J_0/\Delta J$ which they termed the spin-glass phase. For higher values of the parameter a ferromagnetic phase with long-range order resulted. A general review of theoretical work on spin-glasses has been given by Sherrington (1976).

It is of interest to investigate a short-range force model using a more reliable approach than the mean-field approximation, and we shall consider the development of series expansions particularly at high temperatures. This approach was used by Rapaport (1972a,b) for a random-bond model, but his treatment was confined to a ferromagnetic model with positive interactions. We shall consider a simple lattice model with N Ising spins having random nearest-neighbour interactions with equal probability of being $\pm J$.

Let us first summarize the treatment of the more general Ising problem in which an i–j bond of the lattice has interaction J_{ij}. The Hamiltonian is

$$\mathcal{H} = -\sum_{i,j} J_{ij}\sigma_i\sigma_j - mH\sum_i \sigma_i \qquad (1)$$

where i, j refer to the nearest-neighbour bonds of the lattice, and the σ_i can take values ± 1. The partition function in zero field can be calculated in the standard manner (e.g. Domb 1974)

$$Z_N(\beta, 0) = \langle \exp(-\beta\mathcal{H})\rangle = \sum \prod_{\langle ij\rangle} (\cosh K_{ij} + \sigma_i\sigma_j \sinh K_{ij}) \qquad (K_{ij} = \beta J_{ij}, \beta = 1/kT) \quad (2)$$

the product being taken over all nearest-neighbour pairs $\langle ij\rangle$ of the lattice, and the sum over the 2^N values of the σ_i. Thus

$$\ln Z_N(\beta, 0) = \sum_{\langle ij\rangle} \ln \cosh K_{ij} + \sum_{\sigma_i=\pm 1} \ln \prod_{\langle ij\rangle} (1 + \sigma_i\sigma_j w_{ij}) \qquad (w_{ij} = \tanh K_{ij}). \qquad (3)$$

The terms in (3) can be split into a 'one-dimensional' type of contribution

$$N \ln 2 + \sum_{\langle ij\rangle} \ln \cosh K_{ij} \qquad (4)$$

and a configurational series corresponding to each star embedding on the lattice. The stars can be classified according to *topology* (i.e. a star graph with all two degree vertices suppressed) and the first few topologies are shown in figure 1.

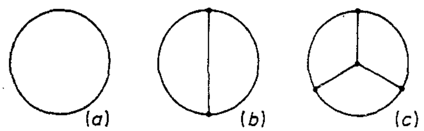

Figure 1. Some representative topologies. (a) polygon ($c = 1$); (b) θ-topology ($c = 2$); (c) α-topology ($c = 3$).

A star graph with a particular set of two degree vertices having this toplogy is termed a *realization* of the topology (Martin 1974). For each topology we define *bondings* (Domb 1972a) in which each edge of the topology has a certain multiplicity (figure 2). With each bonding we associate a weight w, and once this is known the contribution of

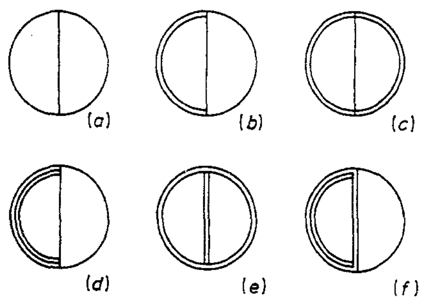

Figure 2. Typical bondings of a θ-topology with their weights: (a) $w = 0$; (b) $w = -1$; (c) $w = 0$; (d) $w = 0$; (e) $w = 2$; (f) $w = 1$.

any particular realization of the topology can be written down immediately for this bonding. Thus for example for the star in figure 3 the contribution corresponding to the bonding in figure 2(*f*) is

$$w_{21}^3 w_{15}^3 w_{54}^3 w_{26}^2 w_{64}^2 w_{23} w_{34}. \tag{5}$$

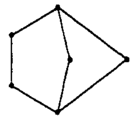

Figure 3. A realization of the θ-topology with 7 edges.

There are simple rules which enable one to identify bondings with $w=0$ and hence eliminate them (Domb 1976); the most important is that all bondings with any odd vertices have $w=0$ (e.g. figures 2(*a*), (*c*), (*d*)).

We now proceed to a stochastic model by averaging $\ln Z_N$ over the probability distribution of bond strengths, and since we have chosen a distribution with equal probabilities of the interaction being positive and negative, all terms involving odd powers of w cancel to zero. Hence, we can confine attention to bondings in which each edge of the topology has even multiplicity.

It is a straightforward matter to derive terms of the configurational series expansion for various two and three dimensional lattices; for example, for the FCC lattice the first few terms are

$$-4w^6-\tfrac{33}{2}w^8-12w^{10}+291w^{12}. \tag{6}$$

We defer the analysis and discussion of such expansions to a subsequent publication, and confine attention at present to a general assessment of asymptotic contributions.

The contribution of an r-gon with weak lattice constant p_r is

$$p_r(-\tfrac{1}{2}w^{2r}+\tfrac{1}{3}w^{3r}-\tfrac{1}{4}w^{4r}\dots). \tag{7}$$

p_r is asymptotically of the form (Martin *et al* 1967)

$$p_r \sim \mu^r r^{-h} \tag{8}$$

where μ is the self-avoiding walk limit, $h\sim 2\frac{1}{2}$ in two dimensions and $h\sim 2\frac{3}{4}$ in three dimensions; hence the contribution to the coefficient of w^{2n} of terms other than the first in (7) can be neglected for large n. The contribution of the first term is negative, and of the form $-\frac{1}{2}\mu^n n^{-h}$.

The first bonding of a θ-topology which contributes is that of figure 2(*e*) (all the others in figure 2 give zero contributions). Hence a realization of the θ-topology with r, s, t links in its edges contributes

$$2(r,s,t)_\theta w^{2r+2s+2t} \tag{9}$$

from this bonding, where $(r,s,t)_\theta$ is the weak lattice constant of the realization. The contribution of all such realizations to the term in w^{2n} is then

$$2\sum(r,s,t)_\theta, \qquad (r+s+t=n) \tag{10}$$

and this has the asymptotic value $A\mu^n n^{-h+1}$ (Domb 1972a and later numerical estimates). Therefore this term is more significant asymptotically than the polygon term as is already evident in the series (6).

However, higher-order graphs contribute alternately negatively and positively, and it is difficult to predict an asymptotic pattern of behaviour without a more detailed investigation. By analogy with the standard Ising model a self-avoiding walk type of approximation (Domb 1970) would indicate a singularity at

$$w^2 = \frac{1}{\mu}, \qquad w = 1/\mu^{1/2} \tag{11}$$

We now consider the derivatives of $\ln Z_N(\beta, H)$ with respect to magnetic field H, and these can conveniently be expressed in terms of spin-correlation functions. Using the transformation

$$\exp(\beta m H \sigma_i) = \cosh \beta m H + \sigma_i \sinh \beta m H = \cosh \beta m H (1 + \sigma_i \tau) \qquad (\tau = \tanh \beta m H) \tag{12}$$

it can be shown that for any particular model (Domb 1970, equation (31))

$$\frac{1}{2!}\frac{\partial^2}{\partial \tau^2} \ln Z_N(\beta, J, 0) = \tfrac{1}{2}N + \sum_{\text{pairs}} \langle \sigma_i \sigma_j \rangle \tag{13}$$

$$\frac{1}{4!}\frac{\partial^4}{\partial \tau^4} \ln Z_N(\beta J, 0) = \tfrac{1}{4}N + \sum_{\text{quadruplets}} \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle - \tfrac{1}{2} \sum_{\text{pairs}} \langle \sigma_i \sigma_j \rangle^2 \tag{14}$$

where

$$\langle f(\sigma_i, \sigma_j, \ldots) \rangle = \sum_{i,j} f(\sigma_i, \sigma_j, \ldots) \exp-(\beta \mathscr{H})/Z_N(\beta, 0). \tag{15}$$

The first term on the right-hand side of (13) represents the contribution of uncoupled spins. The correlation between spins at any two points which enters into the second term can be evaluated by introducing a fictitious extra bond J' between the two points, calculating the partition function, and allowing J' to tend to zero (Domb 1972a). We then find that the graphs which determine the series expansion for the pair correlation are derived from stars by eliminating an edge between two points (figure 4); and the only bondings of the corresponding topologies which need be considered are those in which the broken line (representing the eliminated edge J') is single.

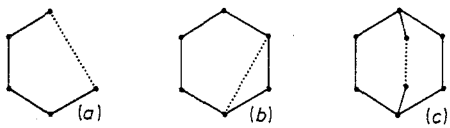

Figure 4. Graphs which contribute to the spin-pair correlation function and magnetic susceptibility.

This means that the multiplicity of at least one of the other edges must be odd in order to make the vertices even. Hence, when we pass to a stochastic model all graphs average to zero. Therefore, as far as the high-temeperature phase of the stochastic model is concerned, *all spin-pair correlations are zero and the magnetic susceptibility corresponds to uncoupled spins.*

Proceeding to the fourth derivative with respect to magnetic field, the first term on the right-hand side of (14) represents the contribution of uncoupled spins; the second term representing 4-point correlations can be evaluated by introducing two fictitious bonds J', J'' between two points, calculating the partition function and allowing J', J'' to tend to zero. The graphs which determine series expansions for 4-point correlations are stars in which two edges between pairs of points have been eliminated (figure 5). Some of these graphs are disjoint and are cancelled by graphs in the third term of the right-hand side of (14), since the expansion of $\ln Z_N$ must involve only connected graphs. The only remaining graphs from this third term are overlaps of pairs of correlation graphs which contribute to $\langle \sigma_i \sigma_j \rangle$.

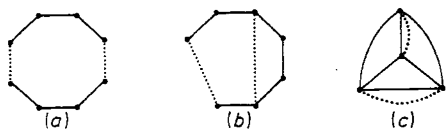

Figure 5. Graphs which contribute to the 4-point correlation function. (a) Disjoint; (b) and (c) connected.

When we pass to a stochastic model all of the 4-point graphs average to zero because of bonds of odd multiplicity, as before. The only overlapping pair correlation graphs giving a contribution are those which overlap exactly (figure 6). The contribution of these graphs is known exactly in terms of the standard Ising model. Thus is a_n is the nth coefficient of the susceptibility series for the standard Ising model, the contribution to the fourth derivative of $\ln Z_N$ with respect to H is

$$-\tfrac{1}{2}\sum a_n w^{2n} = -\tfrac{1}{2}\chi_0^{\mathrm{I}}(w^2), \tag{16}$$

where $\chi^{\mathrm{I}}(w)$ is the susceptibility of the Ising model. This has a singularity at

$$w = w_c^{1/2} \tag{17}$$

where w_c corresponds to the Curie point of the standard Ising model.

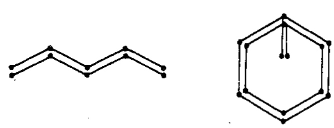

Figure 6. Exact overlap of two spin-pair correlation graphs.

We can proceed similarly for higher derivatives and find that if r is odd, the $2r$th derivative of $\ln Z_N$ is identical with that for uncoupled spins; whilst if r is even configurations in the $2r$th derivative of $\ln Z_N$ can be related to configurations in the rth and lower derivatives of $\ln Z_N^{\mathrm{I}}$ for the standard Ising model, with the first singularity given by (17). It is possible that the true singularity of $\ln Z_N$ in zero field is also given by (17) for which (11) is an approximation.

However, it is not clear whether the observed spin-glass singularities correspond to (17), or whether they are discontinuities arising when the low- and high-temperature phases meet (as must certainly be the case for the susceptibility and $2r$th derivatives for odd r). This could be determined in principle by deriving series expansions for the low-temperature phase. But the lowest energy state is highly degenerate with a finite entropy, and is difficult to define precisely.

We can get some feeling for the low-temperature phase by considering a Bethe lattice of coordination number q (Domb 1960) having no closed circuits. Here the lowest energy state is uniquely defined once a single spin is specified, the orientations of a pair of spins having the same sign when the bond is ferromagnetic, and opposite signs when the bond is antiferromagnetic. In zero field the model is then isomorphic with the Ising model for this pseudo-lattice, and the discontinuity in specific heat occurs when

$$w = 1/(q-1). \tag{18}$$

This value gives a temperature significantly higher than (17) especially for larger q.

The susceptibility and higher derivatives with respect to H can be calculated for the Bethe lattice, and the behaviour at very low temperatures is similar to that of an antiferromagnet. However, if we are to get any idea of the true position and nature of the singularity in the low-temperature phase we must proceed to a higher order closed form approximation like that of Kikuchi (see e.g. Burley 1972) which can take the degeneracy of the lowest energy state into account.

These considerations also suggest an order parameter ζ different from that used by previous authors with a simple physical interpretation. Let $\epsilon(J_p)$ represent the energy of a particular bond. Define

$$\zeta = \lim_{|p-q|\to\infty} \langle \epsilon(J_p)\epsilon(J_q)\rangle. \tag{19}$$

At sufficiently low temperatures where the spins are organized to give maximum energy this should be non-zero, whereas in the high-temperature phase it is zero. Such energy–density energy–density correlations have been considered for the standard Ising model (e.g. Hecht 1967). We can look upon a spin-glass phase as one with no long-range spin–spin correlation, but with a long-range energy–density energy–density correlation.

The treatment of the high-temperature phase can readily be extended to the D vector model using appropriate eigenfunction expansions to derive the partition functions for star topologies (Domb 1972b, 1976). However, the usual difficulty arises in defining the low-temperature phase because of the infinite entropy at $T=0$.

As we have indicated, more precise information on the nature of critical behaviour in a spin-glass can best be obtained by numerical calculations for specific two and three dimensional lattices. A programme which makes use of the extensive star-lattice constant data available has therefore been initiated.

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