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Anisotropic spin-glasses with broken replica symmetry

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Abstract. A simple mechanism of replica symmetry breaking for spin-glass, as suggested by Parisi, has been used to solve the anisotropic spin-glass model of Sherrington and Ghatak. Temperature variation of the correlation parameters and the resulting variations with the temperature of the thermodynamic quantities like internal energy, specific heat and entropy have been evaluated. It is found that the anisotropy has considerable effect on the properties of the spin system. At low temperatures, the specific heat varies as T^2. However, the entropy is positive for temperatures above 0·1°K, which is a considerable improvement on the results of Sherrington and Ghatak. The results are expected to be in good agreement with experiment or computer simulation studies near transition temperatures.

Keywords. Replication procedure; spin-glass order parameter; replica symmetry breaking; critical temperature.

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1. Introduction

Sherrington and Kirkpatrick (SK) (1975, 1978) have formulated a solvable infinite ranged model of spin-glass which consists of long range exchange forces coupling all pairs of spins in the system. This is the analogue of the Curie-Weiss mean field theory of ferromagnets. SK have followed the replica theory suggested by Edward and Anderson (1975). The Hamiltonian is of N interacting Ising spins; $\mathscr{H} = -\sum_{(ij)} J_{ij} S_{ij} S_{iz}$, (ij) denoting the inequality between i and j. i and j take the values 1, 2, ... N and the spin operators S_z can take the values ± 1 only. The distribution of the values of the bonds is a Gaussian with variance $1/N$.

The difficulty of the problem lies in the quenched nature of the disorder. To circumvate this difficulty, the mathematical identity in $Z = \lim_{n\to 0} (Z^n - 1)/n$ is used for the partition function $Z \cdot Z^n$ is again decomposed as a finite product like $Z^n = \prod_{\alpha=1}^{n} Z_\alpha$. α is the dummy label taking the values $1, 2, \ldots$ to n.

All the α's are treated like the identical free replicas of the real system having exactly the same disorder. The logarithmic identity converts the averaging of the free energy over the possible disordered systems to an averaging of the partition function. Thus the replica method averages the free energy and not the partition function Z to convert the quenched problem into an annealed one. There remains, therefore, only the evaluation of the thermal trace over the exponential of an effective Hamiltonian.

While finding out the internal energy for the system, SK have defined the spin-glass order parameter $q^{\alpha\beta} = \langle s_z^\alpha s_z^\beta \rangle$ which is averaged to give the correlation parameter $q^{\alpha\beta} = q$ for $\alpha \neq \beta$ and $q^{\alpha\beta} = 0$ for $\alpha = \beta$. A non-zero q will indicate the existence of a spin-glass phase.

After taking the thermodynamic limit $N \to \infty$ first and then letting $n \to 0$ next, SK have calculated the internal energy, the specific heat and the entropy in terms of q. At higher temperatures, when $q = 0$ is a solution, these results agree with their results of computer simulations. But with the onset of spin-glass phase having non-vanishing q, the results for energy and specific heat differs and the differences continue to grow with decrease in temperature. The disagreements are much pronounced as the temperature is close to zero. At absolute zero, the entropy turns out to be $-k/2\pi$. Such a negative value is unphysical.

As a remedy to this failure of the theory, some form of replica symmetry breaking is essential in the spin-glass-phase. Parisi (1979) suggested a spontaneous symmetry breaking in which the variables $q^{\alpha\beta}$ assume one value within one replica and a different value in another. In §2, we give the formulae and the results for this simple scheme which agree well with computer simulation results till about $T \simeq 0{\cdot}15$ (with transition temperature taken as 1°K). Furthermore, the results of Parisi in the temperature range of 0·15 to 0·4 agree with the theoretical results of Thouless *et al* (1977).

In the meantime, Sherrington and Ghatak (SG) (1977) have applied SK's method to an interacting spin system which include crystal field effects. They have followed SK's method using the same Edward–Anderson replication procedure and calculated the free energy, the internal energy and the specific heat for different anisotropy parameters. The results are very similar to the SK's theoretical results. Not only their specific heat is linear in T in the low temperature range, but also the entropy comes out to be negative (Deo and Mishra 1984) and equals $(-k/2\pi)$ at absolute zero. Hence in the case of a spin system with anisotropy, one can also postulate the existence of a spontaneous symmetry breaking. In §3 we carry out the modification of Sherrington and Ghatak's model following the simple scheme of Parisi. A detailed calculation of the correlation parameters is presented and the thermodynamic observables in the low and high temperature regions are evaluated for three different values of anisotropy parameter. In §4, the results obtained are discussed.

2. Parisi's results

First we outline the method of calculation and present the results of Parisi's model. It may be easily seen from the SK model that when the thermodynamic limit $N \to \infty$ is taken, the free energy F reduces to

$$\beta F = \frac{1}{4}\beta^2 + \max\left[\lim_{n\to 0}\frac{1}{n}\sum_{(\alpha\beta)}\frac{\beta^2}{4}(q^{\alpha\beta})^2 - \frac{1}{n}\ln \mathrm{Tr}\exp\left(\beta^2\sum_{(\alpha\beta)} q^{\alpha\beta}S^\alpha S^\beta\right)\right]$$

where $$\beta = \frac{1}{kT}. \tag{1}$$

The n replicas are further subdivided into groups each containing m replicas. The symmetry is broken by hypothesising that $\langle q^{\alpha\beta} \rangle = (p+t)$, if replicas (α, β) belong to the same subgroup and equals p, only if (α, β) are in different groups. With this simple scheme, in the limit $n \to 0$, the free energy is given by

$$\beta F(p,t,m) = -\frac{1}{4}\beta^2[1 + mp^2 + (1-m)(p+t)^2 - 2(p+t)] + \ln 2$$
$$-\frac{1}{m}\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp(-\tfrac{1}{2}z^2) \ln\left[\int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp(-\tfrac{1}{2}y^2) \cosh^m \Sigma\right] \tag{2}$$

where $\Sigma = \beta p^{1/2} z + \beta t^{1/2} y.$

At the maximum,

$$\frac{\partial F}{\partial m} = \frac{\partial F}{\partial p} = \frac{\partial F}{\partial t} = 0.$$

Using this condition one obtains the following equations for p, t and m. With

$$R(z) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right) \cosh^m \Sigma$$

$$p = 1 - t(1-m) - \frac{1}{\beta\sqrt{p}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}}$$
$$\times \exp\left(-\frac{y^2}{2}\right) z \tanh \Sigma \cosh^m \Sigma / R(z). \tag{3a}$$

$$(1-m)t = 1 - p(1-m) - \frac{1}{\beta\sqrt{t}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}}$$
$$\times \exp\left(-\frac{z^2}{2}\right) \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right) y \tanh \Sigma \cosh^m \Sigma / R(z). \tag{3b}$$

$$m = \frac{4}{\beta^2 t(t+2p)}\left[\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right) \cosh^m \Sigma\right.$$
$$\left.\times \ln(\cosh\Sigma)/R(z) - \frac{1}{m}\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \ln R(z)\right]. \tag{3c}$$

Using computer these above equations have been solved self-consistently. The free energy is then obtained from (2). The results for p, t and m at different temperatures have been plotted in figures 4–6. We have not found such plots in the existing literature. It is seen that near the critical temperature ($T_g = 1$), $p \simeq 1/3\,\tau$, $t \simeq 2/3\,\tau$ and $m \simeq \tau$ with $\tau = T_g - T$; in agreement with the calculation of Parisi. We should note here that we use the Boltzmann constant $k = 1$.

The internal energy $U(T)$, the specific heat $C_v(T)$, the entropy $S(T)$ have been calculated using the free energy equation. They are computed numerically and are plotted against temperature in figures 1–3. It is seen that the functions $U(T)$ and $C_v(T)$ are in excellent agreement with the computer simulations. As has already been found out by Parisi in the region $0.2 < T < 0.4$, the internal energy is given by $U(T) \simeq U_0 + \frac{1}{3}AT^3$ with $A \simeq 1.4$ and $U_0 \simeq -0.764$. So the specific heat is quadratic in the same region, *i.e.*, $C_v(T) \simeq AT^2$. The entropy is given by $S(T) \simeq \frac{1}{2}A^2T^2$. These results are

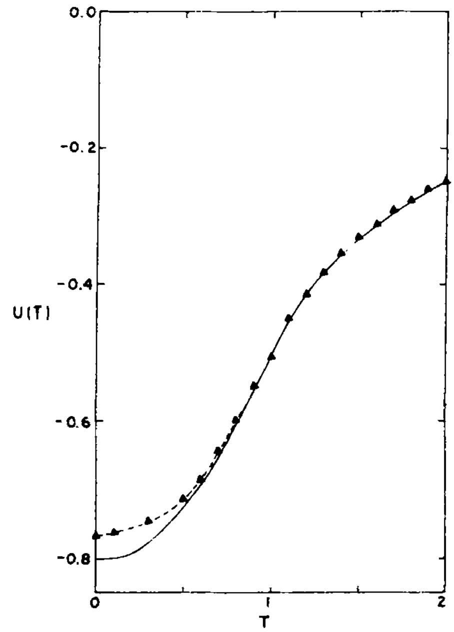

Figure 1. Internal energy $U(T)$ as a function of temperature T. The solid line gives SK's variation, the broken line being that of Parisi's prediction. The (▲)'s give the Monte Carlo data.

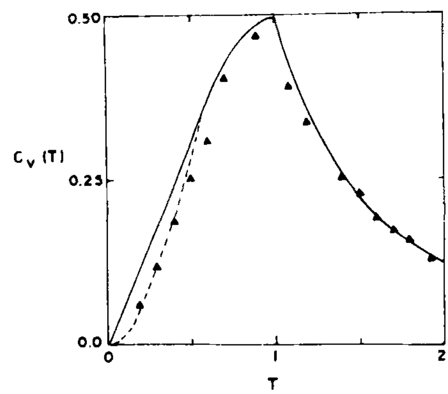

Figure 2. Specific heat $C_v(T)$ as a function of temperature. The solid and the dashed lines represent the respective theoretical results of SK and Parisi; the (▲)'s being the computer simulation results.

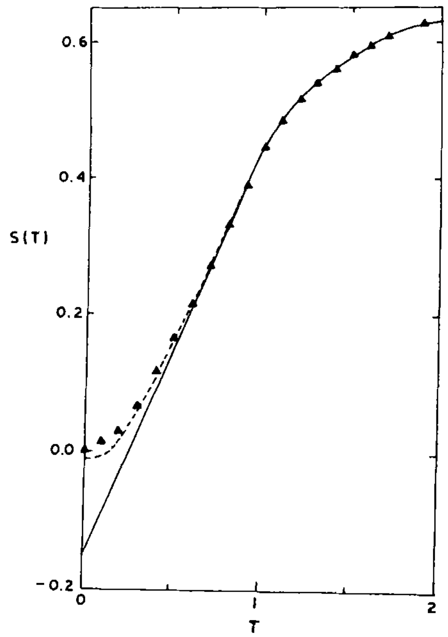

Figure 3. The variation of the entropy $S(T)$ with temperature. SK's and Parisi's results are given by the solid line and the dashed line respectively whereas the (▲)'s denote the Monte Carlo simulations.

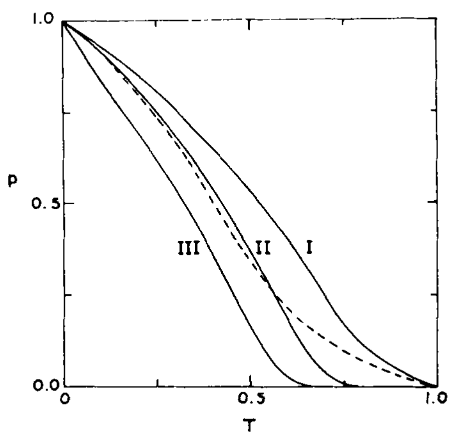

Figure 4. Temperature dependence of p for different values of D = 5, 0 and −0·5 (I, II, III). The dashed line gives the values of p from Parisi's free energy.

more in agreement with TAP result than the original SK solutions. Therefore it is to be concluded that Parisi's method tends to reproduce the correct results and are reliable for all temperatures above $0{\cdot}2T_g$.

At lower values of T, our calculations definitely agree with the Monte Carlo simulations for the function $U(T)$ and $C_v(T)$. At absolute zero, the internal energy is

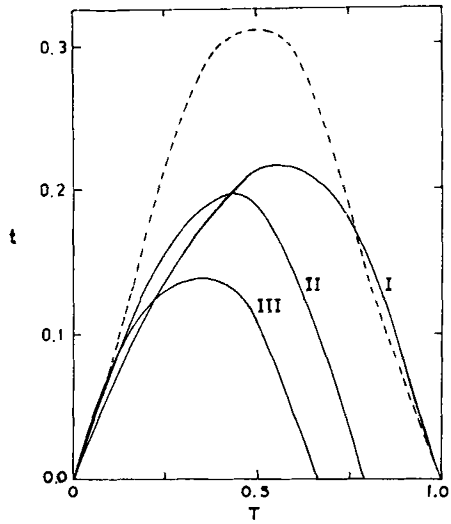

Figure 5. t as a function of temperature where the solid lines (I, II, III) represent the respective variations for $D = 5$, 0 and $-0{\cdot}5$. The broken line gives the same obtained from Parisi's free energy.

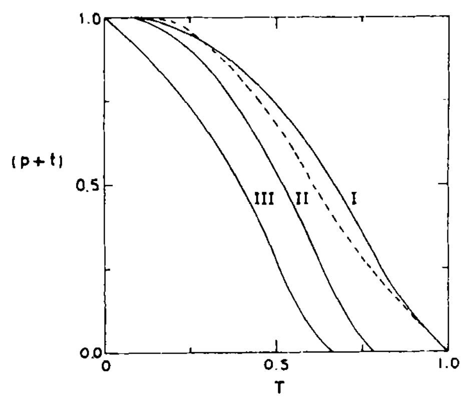

Figure 6. Variation of $(p+t)$ with temperature by the three solid curves (I, II, III) for $D = 5$, 0 and $-0{\cdot}5$. The dashed line is Parisi's theoretical result.

given by $U(0) \simeq -0{\cdot}765$. But unfortunately the entropy becomes negative for $T \leqslant 0{\cdot}1$ and $S(0) \simeq -0{\cdot}01$.

The failure of this simple scheme regarding the value of the entropy near absolute zero has led Parisi to suggest that there is not one but a series of microtransitions as the spin-glass is heated from zero to the critical temperature. By introducing continuous symmetry breaking he has been able to solve the problem of negative entropy at $T = 0°\mathrm{K}$. What is treated as continuous is the correlation function

$$q = q(x) = \langle S_z^\alpha S_z^\beta \rangle = \langle \overline{S_z} \rangle^2$$

In the SK model the values of S_z are only ± 1 and there is no anisotropy. In the Sherrington and Ghatak model on the other hand S_z can take three values ± 1 and 0. The zero component introduce additional factors in the free energy (Ghatak and Sherrington 1977). Furthermore, due to anisotropy, there is another spin correlation factor

$$r = \langle (\overline{S_z})^2 \rangle. \tag{4}$$

This can be taken to be unaltered when there is single symmetry breaking as both S_z's of equation belong to the same replica. In the continuous case this is not bound to remain constant.

For these reasons we have been unable to generalise to the continuous symmetry breaking scheme of Parisi. In any event, the study of the thermodynamic quantities near the transition point is important. Therefore, we think it is worthwhile to calculate these properties of anisotropic spin-glass system with a single symmetry breaking mechanism.

3. Replica symmetry breaking in Sherrington-Ghatak model

In Sherrington-Ghatak model, crystal field effects are studied in an anisotropic spin-glass system. The above authors followed SK calculations and have reported their results for the internal energy, specific heat and entropy. Their results will be correct for a temperature higher than the spin-glass temperature but could differ appreciably for low temperature near and below the transition temperature.

The SG Hamiltonian for an anisotropic system of N spins interacting with each other *via* a random exchange interaction, is given by

$$\mathscr{H} = -\sum_{(ij)} J_{ij} S_{iz} S_{jz} - D \sum_i S_{iz}^2. \tag{5}$$

where z is the anisotropy axis and S_{iz} takes three values -1, 0 and $+1$. J_{ij} as usual has zero diagonal elements and the bonding is a random Gaussian with variance $1/N$ as before. D is the anisotropic parameter which influences all physical parameters specially the spin-glass temperature T_g. The averaged partition function is given by

$$\overline{Z^n} = \mathrm{Tr} \exp\left[\frac{\beta^2 J^2}{2N} \sum_{(ij)} \sum_{\alpha\beta} S_{iz}^\alpha S_{jz}^\alpha S_{iz}^\beta S_{jz}^\beta + D\beta \sum_{i\alpha} (S_{iz}^\alpha)^2 \right]$$

The mean field parameters in the replicated system are the correlations

$$r^\alpha = \langle (S_{iz}^\alpha)^2 \rangle_n,$$
$$q^{\alpha\beta} = \langle (S_{iz}^\alpha S_{iz}^\beta) \rangle_n, \quad \alpha \neq \beta \tag{7}$$

with the brackets denoting the thermal average over the n replicas. In SG's model at the extremum of the free energy,

$$r = \langle (\overline{S_z})^2 \rangle, \quad q = (\langle \overline{S_z} \rangle)^2$$

the bar denoting an average over the quenched randomness. Note the presence of two correlations instead of one in the SK model. Considering the terms with $\alpha = \beta$ and $\alpha \neq \beta$ separately we write,

$$\sum_{(ij)} \sum_{\alpha\beta} S^{\alpha}_{iz} S^{\alpha}_{jz} S^{\beta}_{iz} S^{\beta}_{jz} = \sum_{(ij)} \sum_{\alpha} (S^{\alpha}_{iz})^2 (S^{\alpha}_{jz})^2 + 2 \sum_{(ij)} \sum_{(\alpha\beta)} S^{\alpha}_{iz} S^{\beta}_{jz} S^{\alpha}_{iz} S^{\beta}_{jz}$$

Next we use the mean-field approximations as

$$\sum_{(ij)} \sum_{\alpha} (S^{\alpha}_{iz})^2 (S^{\alpha}_{jz})^2 \simeq N \sum_{i\alpha} \left[r(S^{\alpha}_{iz})^2 - \frac{r^2}{2} \right]$$

$$\sum_{(ij)} \sum_{(\alpha\beta)} S^{\alpha}_{iz} S^{\beta}_{iz} S^{\alpha}_{jz} S^{\beta}_{jz} \simeq N \sum_{i} \sum_{(\alpha\beta)} \left[q^{\alpha\beta} S^{\alpha}_{iz} S^{\beta}_{jz} - \frac{(q^{\alpha\beta})^2}{2} \right]$$

and finally the averaged partition function

$$\overline{Z^n} = \exp\left(\tfrac{1}{4} N n \beta^2 \tilde{J}^2\right) \int \pi_{(\alpha\beta)} \frac{\mathrm{d}q^{\alpha\beta}}{\sqrt{2\pi}} \exp[-Nf(q)] \tag{8}$$

where,

$$f(q) = \tfrac{1}{4} \beta^2 \tilde{J}^2 \left[\sum_{(\alpha\beta)} (q^{\alpha\beta})^2 + nr^2 \right] - \ln \operatorname{Tr} \exp \left[\frac{\beta^2 \tilde{J}^2}{2} \sum_{i} \sum_{(\alpha\beta)} q^{\alpha\beta} S^{\alpha}_{iz} S^{\beta}_{iz} + \frac{\beta^2 \tilde{J}^2}{2} r \sum_{i} \sum_{\alpha} (S^{\alpha}_{iz})^2 + D\beta \sum_{i} (S^{\alpha}_{iz})^2 \right]. \tag{9}$$

This is Sherrington and Ghatak's result. From this result, one can easily obtain all the thermodynamic properties like energy, specific heat, entropy and susceptibility. The specific heat will vary linearly below the spin-glass transition temperature. In general, the behaviour of the system will be same as in the SK model. From the nature of the deviation of the SK results from computer simulation values, it can be informed that the predictions from the above equation will not be reliable near the transition temperature. As our previous calculation showed, near and below the transition temperature, single symmetry breaking yields accurate values of thermodynamic quantities in the SK model. The effect of this breaking in the anisotropic case is examined below.

The break down of replica symmetry affects the two terms containing q in the expression for $f(q)$. SG value of these terms are

$$\sum_{(\alpha\beta)} (q^{\alpha\beta})^2 = n(n-1)q^2$$

and

$$\sum_{(\alpha\beta)} q^{\alpha\beta} S^{\alpha}_{iz} S^{\beta}_{iz} = q \left[\left(\sum_{\alpha} S^{\alpha}_{iz} \right)^2 - \sum_{\alpha} (S^{\alpha}_{iz})^2 \right]$$

These values will change now. We consider the n replicas to be divided into M subgroups each having m replicas. So q now can have two values; $(p+t)$ when α, β are the members of the same group and (p) when α, β belong to different groups. The new expressions are

$$\sum_{\alpha\beta}(q^{\alpha\beta})^2 = [n(m-1)(p+t)^2 + n(n-m)p^2]$$

and

$$\sum_i \sum_{\alpha\beta} q^{\alpha\beta} S^{\alpha}_{iz} S^{\beta}_{iz} = \left[(q-p)M\left(\sum_{\alpha=1}^{m} S^{\alpha}_{iz}\right)^2 + p\left(\sum_{\alpha=1}^{n} S^{\alpha}_{iz}\right)^2 - q\sum_{\alpha=1}^{n}(S^{\alpha}_{iz})^2\right]$$

Then using the integral equality

$$\exp(\lambda a^2) = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp\left[-\frac{z^2}{2} + (2\lambda)^{1/2} az\right]$$

we immediately obtain the general expression for the free energy (for $\tilde{J} = 1$) in the limit $n \to 0$

$$F = -\tfrac{1}{4}\beta^2[mp^2 - r^2 + (1-m)(p+t)^2]$$
$$-\frac{1}{m}\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\ln\left[\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)\right.$$
$$\left.\mathrm{Tr}\,(\exp\{\alpha S^2_{iz} + \beta S_{iz}(y\sqrt{t} + z\sqrt{p})\})^m\right] \tag{10}$$

where $$\alpha = \frac{\beta^2}{2}[r - (p+t)] + D\beta. \tag{10a}$$

The traces are calculated summing over all three possible values of S_z. The free energy expression which will be used to determine the thermodynamic variables is

$$\beta F = -\tfrac{1}{4}\beta^2[mp^2 - r^2 + (1-m)(p+t)^2]$$
$$-\frac{1}{m}\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\ln\left[\int_{-\infty}^{+\infty}\cdot\frac{dy}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)\right.$$
$$\left.\times\{1 + e^{\alpha}2\cosh(\beta\sqrt{p}z + \beta\sqrt{t}y)\}^m\right]. \tag{11}$$

For the extremum of the free energy

$$\frac{\partial F}{\partial m} = \frac{\partial F}{\partial p} = \frac{\partial F}{\partial t} = \frac{\partial F}{\partial r} = 0.$$

The self-consistent equations from which p, t, r and m are to be found out are

$$r = \int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)$$
$$2\cosh\Sigma\,(e^{-\alpha} + 2\cosh\Sigma)^{m-1}/R_{\alpha}(z). \tag{12a}$$

$$p+t=\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)$$
$$\times 4\sinh^2\Sigma(e^{-\alpha}+2\cosh\Sigma)^{m-2}/R_\alpha(z). \tag{12b}$$

$$p=\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\left[\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)\right.$$
$$\left.\times 2\sinh\Sigma(e^{-\alpha}+2\cosh\Sigma)^{m-1}/R_\alpha(z)\right]^2. \tag{12c}$$

$$m=\frac{4}{\beta^2t(t+2p)}\left[\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\int_{-\infty}^{+\infty}\frac{dy}{\sqrt{2\pi}}\right.$$
$$\times\exp\left(-\frac{y^2}{2}\right)(e^{-\alpha}+2\cosh\Sigma)^m\ln(e^{-\alpha}+2\cosh\Sigma)/R_\alpha(z)$$
$$\left.-\frac{1}{m}\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\ln\{R_\alpha(z)\}\right]. \tag{12d}$$

where $\Sigma=\beta p^{1/2}z+\beta t^{1/2}y$

and
$$R_\alpha(z)=\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)(e^{-\alpha}+2\cosh\Sigma)^m. \tag{13}$$

As a check, it will be noted that the above expressions for $(p+t)$ and r reduce to SG's results (q and r) for $m=0$. The values of t, as it should, also reduce to zero. For sufficiently high temperatures, the solutions for the above equation give $p=0=t=m$ and (12a) reduces to

$$r=\frac{2}{\exp(-\alpha_0)+2}\quad\text{with}\quad\alpha_0=\frac{\beta^2r}{2}+D\beta. \tag{14}$$

As r occurs on both the sides of this equation, it has to be solved self-consistently to obtain r. With decrease of temperature, both p and m differ from zero and then gradually increase and attain the value one. However, t at first increases from zero, exhibits a maximum and then reduces to zero at absolute zero.

Near the spin-glass temperature T_g, (12a) and (12b) lead to $\beta_g r_g=1$. So we obtain

$$T_g=1/[1+\tfrac{1}{2}\exp(-0{\cdot}5\beta_g(1+2D))]. \tag{15}$$

Thus the spin-glass temperature is quite different for different values of D and decreases as the value of D is lowered.

The internal energy $U(T)$, the specific heat $C_v(T)$ and the entropy $S(T)$ are easily evaluated from the free energy equation. Expressions for them are given below (with $\beta=1/T$)

$$U(T)=\frac{1}{\beta^2}\frac{\partial}{\partial T}(-\beta F),$$
$$=-\frac{\beta}{2}[r^2+mt(t+2p)-(p+t)^2]-Dr. \tag{16}$$

$$C_v(T) = \frac{\partial U(T)}{\partial T},$$

$$= \frac{\beta^2}{2}[r^2 - (p+t)^2 + mt(t+2p)$$

$$-\frac{\beta}{2}\left[2\left(r + \frac{D}{\beta}\right)\frac{\partial r}{\partial T} - 2\{p + t(1-m)\}\frac{\partial p}{\partial T}\right.$$

$$\left. - 2(p+t)(1-m)\frac{\partial t}{\partial T} + t(t+2p)\frac{\partial m}{\partial T}\right]. \tag{17}$$

$$S(T) = \frac{\beta^2}{4}[\{r - (p+t)\}\{r - 3(p+t) - 2\} - 3mt(t+2p)]$$

$$+ 1\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \ln\{R_\alpha(z)\}$$

$$+ \beta^2[r - (p+t) + DT]e^{-\alpha}\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \Big/ R_\alpha(z)$$

$$\times \int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right)(e^{-\alpha} + \cosh\Sigma)^{m-1}. \tag{18}$$

It should be noted that the susceptibility has got two components due to the crystal field effects. Expressions for them have been given by Ghatak and Sherrington (1977). The parallel susceptibility is obtained from free energy as

$$\chi_\parallel(T) = -\left.\frac{\partial^2 F}{\partial H_z^2}\right|_{H_z=0}$$

$$= g^2\mu_B^2\beta[r - (p+t) + mt], \tag{19}$$

where H_z = external magnetic-field in the z-direction. The perpendicular susceptibility is

$$\chi_\perp(T) = -\left.\frac{\partial^2 F}{\partial H_x^2}\right|_{H_x=0}$$

$$= g^2\mu_B^2\beta\int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right)\int_{-\infty}^{+\infty} \frac{\mathrm{d}y}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right)$$

$$\times \frac{[2\{e^{-\alpha} + 2\cosh\Sigma\}^{m-1}M(z)]}{\{R_\alpha(z)\}} \tag{20}$$

with $M(z) = [\alpha\cosh\Sigma - \alpha e^{-\alpha} - \Sigma\cosh\Sigma]/[\alpha^2 - \Sigma^2]$
These have been calculated numerically.

4. Results and discussions

The numerical values of p, t, m and r have been obtained by solving (12b)–(12d) using the computer. The graphs showing their variations with temperature are plotted in figures 4–8 taking $\beta = 1/T$. We have chosen the same three values of $D = 5, 0$ and $-0{\cdot}5$ as has been done by Sherrington and Ghatak.

The critical temperature, as obtained by solving iteratively equation (15), are $T_g = 1$, 0·78 and 0·666 for the values of $D = 5$, 0 and $-0{\cdot}5$ respectively. It is interesting to see that near $T = T_g$, or $\tau = (T - T_g) \to 0$, we get $p \simeq 1/3\tau$ and $t \simeq 2/3\tau$ irrespective of the values of D. These are the same relations as found by Parisi for the isotropic Ising case. Although the nature of variation of the correlation parameters with temperature is quite similar, the values are appreciably different. For the sake of comparison, the results obtained by Parisi are shown by the dashed curves where-ever they exist.

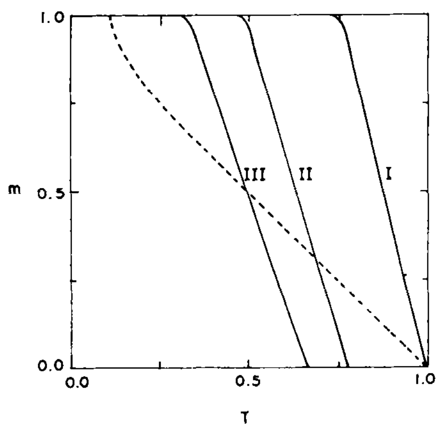

Figure 7. Temperature dependence of m for $D = 5$, 0 and $-0{\cdot}5$ respectively by solid lines (I, II, III) and the dashed line gives that obtainable from Parisi's theoretical prediction.

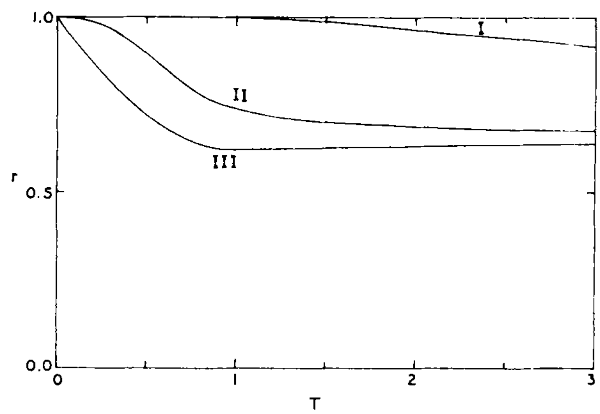

Figure 8. r as a function of temperature. The respective solid lines (I, II, III) present this variation for $D = 5$, 0 and $-0{\cdot}5$.

The nature of variation of the replica breaking parameter m with temperature near T_g is quite different from the isotropic case given by Parisi. Approximately

$$\begin{aligned} m &\simeq 3{\cdot}8(T_g - T) \quad \text{for} \quad D = 5 \\ &\simeq 3{\cdot}2(T_g - T) \quad \text{for} \quad D = 0 \\ &\simeq 2{\cdot}9(T_g - T) \quad \text{for} \quad D = -0{\cdot}5 \end{aligned}$$

The above variations have been found graphically. Furthermore, the value of m increases more sharply to 1 for all values of D than in the isotropic case. The values of the parameter r do not change from those obtained by Sherrington and Ghatak and appear to be quite independent for all temperatures studied.

The functions $U(T)$, $C_v(T)$ and $S(T)$, calculated from the above parameters are plotted against temperature in figures 9, 10 and 11 along side the SG's results. The free

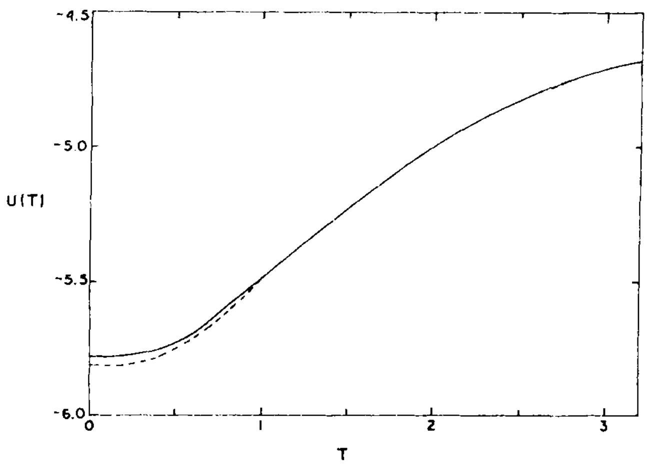

Figure 9a. The internal energy $U(T)$ as a function of temperature for $D = 5$, the broken line is the same for the value of SG.

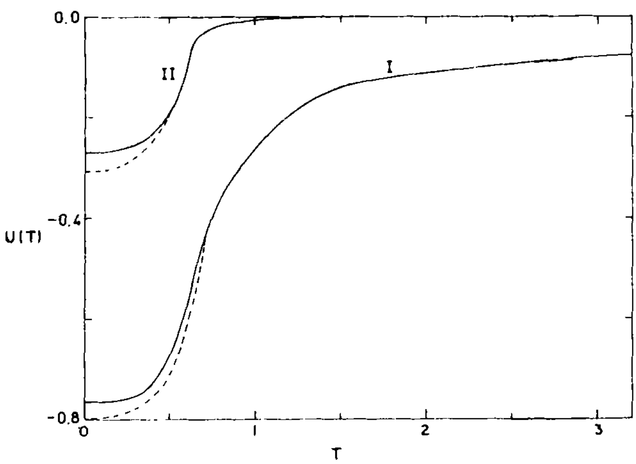

Figure 9b. Temperature dependence of the internal energy $U(T)$ in the solid lines (I, II) for $D = 0$, $-0{\cdot}5$ and the dashed lines represent the same for SG's result.

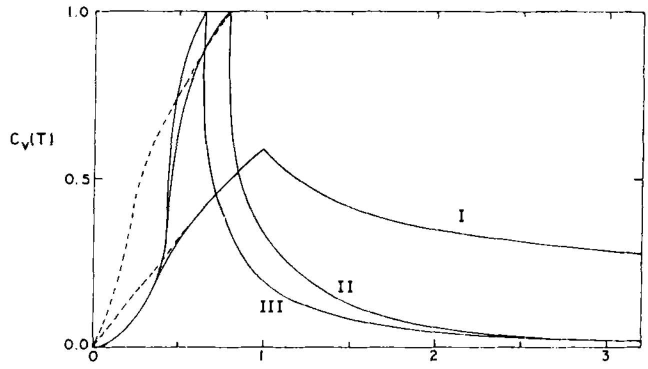

Figure 10. Variation of the specific heat $C_v(T)$ with temperature for $D = 5, 0$ and $-0{\cdot}5$ (I, II, III) whereas the broken line gives the same for SG's results.

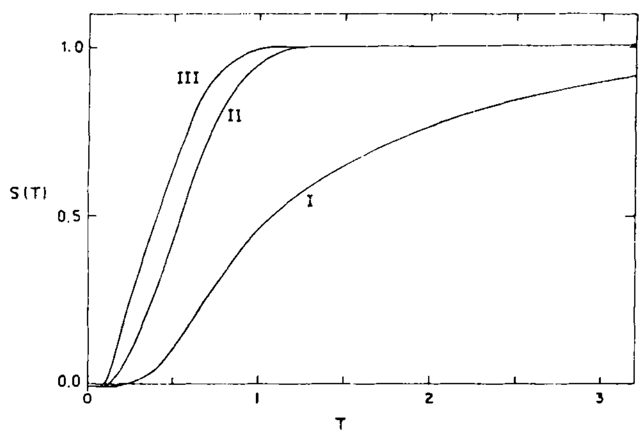

Figure 11. Temperature dependence of the entropy $S(T)$ for $D = 5, 0$ and $-0{\cdot}5$ as given by three solid curves (I, II, III) the dashed line being the same for SG's values.

energy values are higher. Particularly in the region $0{\cdot}2 < T \leqslant 0{\cdot}4$, the internal energy and the specific heat are given as

$$U(T) \simeq U_0 + \tfrac{1}{3}AT^3 \quad \text{and} \quad C_v(T) \simeq AT^2$$

with $A \simeq 1{\cdot}4$ in all cases; but U_0 changes for different D's, being $\simeq -5{\cdot}782$ for $D = 5$, $\simeq -0{\cdot}764$ for $D = 0$ and $\simeq -0{\cdot}267$ for $D = -0{\cdot}5$. The internal energy considerably increases with increase of D. The specific heat is no longer linear in T for small T as obtained by SG, but varies as T^2 in agreement with TAP and Parisi's results. At higher temperatures, the entropy $S(0)$ still becomes negative. It has the approximate values $-0{\cdot}01$ for $D = 0$ and 5; and $-0{\cdot}008$ for the anisotropy constant $D = -0{\cdot}5$.

Regarding the susceptibility, our results are similar to that of Sherrington and Ghatak. There is a slight difference however. The susceptibilities are plotted against temperature in figures 12 and 13. The parallel susceptibility attains the maximum at the

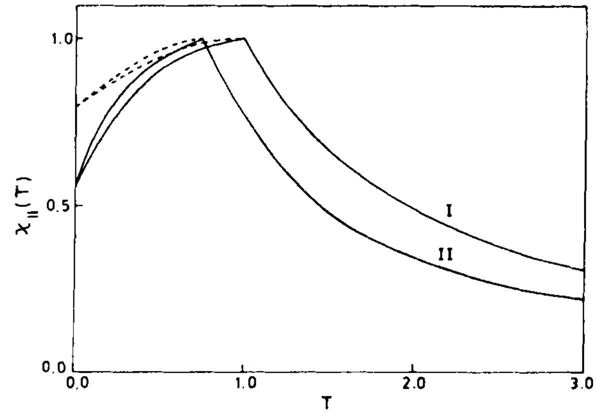

Figure 12. Variation of parallel susceptibility $\chi_{\parallel}(T)$ with temperature for $D = 5$ and 0 (I, II), the broken lines being those of SG's result.

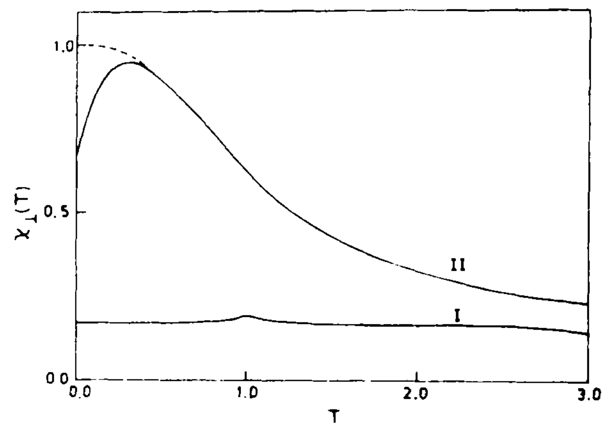

Figure 13. The perpendicular susceptibility $\chi_{\perp}(T)$ as a function of temperature for $D = 5$ and 0 in the solid lines (I, II) and the dashed line gives SG's values.

same temperature as SG but the values towards the lower temperature decrease considerably for both the cases $D = 0$ and $D = 5$. Regarding perpendicular susceptibility, the curve for $D = 5$ exactly coincides with that of SC. The case $D = 0$ shows considerable change at temperatures less than the spin-glass temperature. The cusp is also more pronounced.

Thus we conclude that the calculation based on Parisi's method is a better approximation than Sherrington and Ghatak for the region of $T = 0{\cdot}1$ or $0{\cdot}2$. The results can be compared experimentally with those for $(T_{i_{1-x}}V_x)_2O_3$ or with the computer simulations when they are available.

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