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# First-order transition in a spin-glass model

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**Abstract.** We consider a generalization of the infinite-range Sherrington–Kirkpatrick spin-glass model with arbitrary spin $S$ and the inclusion of crystal-field effects. For integer $S$, replica-symmetric calculations have shown the presence of both continuous and discontinuous transitions and a tricritical point. For $S = 1$, we report a detailed numerical analysis of the replica-symmetric solutions. We locate the first-order boundary and clarify some inconsistencies of the previous analyses. Some analytic asymptotic expansions are used to support the numerical findings.

Ghatak and Sherrington [1] introduced a generalization of the infinite-range Sherrington–Kirkpatrick [2] model of an Ising spin-glass with arbitrary spin $S$ and the inclusion of crystal-field effects. In the replica-symmetric solution, for integer $S$, this generalized model displays both continuous and first-order transitions between the paramagnetic and spin-glass phases. Lage and de Almeida [3] investigated the stability of the replica-symmetric solutions and pointed out some difficulties associated with the analysis of the first-order transition. A more detailed analysis of the critical line, including an application of Parisi's symmetry-breaking scheme, has been published by Mottishaw and Sherrington [4].

In this paper, we take up again the problem of the first-order transition in the spin-1 version of the Ghatak–Sherrington model. We present a detailed numerical study of the replica-symmetric spin-glass solution supplemented by some asymptotic expansions at low temperatures and in the neighbourhood of the tricritical point. Some inconsistencies of the previous works are clearly related to an insufficient numerical analysis of the properties of the spin-glass phase. In the anisotropy($D$)–temperature($T$) phase diagram, Ghatak and Sherrington had already shown the existence of up to three distinct paramagnetic solutions (although only one of them satisfies the stability requirements). In the present paper, we report numerical calculations to show the existence of up to four distinct (and unstable) spin-glass solutions. As in the Sherrington–Kirkpatrick model, there is always a negative eigenvalue of a Hessian matrix. The other eigenvalues, however, may be negative or even complex in large portions of the phase diagram. Since the stability requirements are of no help for the selection of the acceptable spin-glass solution, we propose a criterion which consists in choosing the branch which meets continuously with the spin-glass solution in a region of the phase diagram where there is no chance of ambiguity. Equating the free energies of the paramagnetic and spin-glass solutions, we obtain the first-order boundary. It is remarkable that in this transition region all the stability conditions are violated. In complete agreement with the numerical calculations, an asymptotic analysis is used to

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correct earlier results near the tricritical point. Also, from asymptotic calculations at $T = 0$, we locate the first-order transition at $D = 0.899\,033\,06\ldots$, far from the value $1/\sqrt{2\pi}$, as quoted by previous authors [1, 4].

The spin-glass model of Ghatak and Sherrington is given by the Hamiltonian

$$H = -\sum_{(ij)} J_{ij} S_i S_j + D \sum_{i=1}^{N} S_i^2 \tag{1}$$

where $S_i = 0, \pm 1, \pm 2, \ldots, \pm S$, the $(ij)$ sum is over all distinct pairs of sites, and $D$ is a parameter of anisotropy. The exchange interactions are independent, identically distributed, random variables with a Gaussian probability distribution,

$$p\left(J_{ij}\right) = \left(\frac{N}{2\pi J^2}\right)^{1/2} \exp\left(-\frac{N J_{ij}^2}{2J^2}\right). \tag{2}$$

For $S = 1$, in the $D \to \infty$ limit, we regain the Sherrington–Kirkpatrick model of an Ising spin-glass.

Using the replica method [1, 4], the quenched free energy per site is given by

$$f = \lim_{n \to 0} \frac{1}{n} \min_{(p_\alpha, q_{\alpha\beta})} \left\{ f_n\left[p_\alpha, q_{\alpha\beta}\right] \right\} \tag{3}$$

where

$$f_n\left[p_\alpha, q_{\alpha\beta}\right] = \frac{J^2}{4k_B T} \sum_{\alpha=1}^{n} p_\alpha^2 + \frac{J^2}{2k_B T} \sum_{(\alpha\beta)} q_{\alpha\beta}^2 - k_B T \ln Z_n\left[p_\alpha, q_{\alpha\beta}\right] \tag{4}$$

with

$$Z_n\left[p_\alpha, q_{\alpha\beta}\right] = \mathrm{Tr}_{\{S_\alpha\}} \exp\left\{H_n\left[p_\alpha, q_{\alpha\beta}\right]\right\} \tag{5}$$

and

$$H_n\left[p_\alpha, q_{\alpha\beta}\right] = \left(\frac{J}{k_B T}\right)^2 \sum_{(\alpha\beta)} q_{\alpha\beta} S^\alpha S^\beta + \frac{1}{2}\left(\frac{J}{k_B T}\right)^2 \sum_{\alpha=1}^{n} p_\alpha \left(S^\alpha\right)^2 - \frac{D}{k_B T} \sum_{\alpha=1}^{n} \left(S^\alpha\right)^2 \tag{6}$$

where $(\alpha\beta)$ indicates a distinct pair of replicas ($\alpha \neq \beta$). The extremum conditions are given by $p_\alpha = \left\langle (S^\alpha)^2 \right\rangle$, and $q_{\alpha\beta} = \left\langle S^\alpha S^\beta \right\rangle$, where $\langle \cdots \rangle$ indicates a thermal average with respect to $H_n$ .

In the replica-symmetric ansatz, we have the free energy per site,

$$f = \frac{p^2 - q^2}{4T} - T \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \ln z(x) \tag{7}$$

where

$$z(x) = 1 + 2\exp\left(-\frac{x^* \sqrt{q}}{T}\right) \cosh\left(\frac{x\sqrt{q}}{T}\right) \tag{8}$$

and

$$x^* = \frac{1}{\sqrt{q}}\left(D - \frac{p-q}{2T}\right) \tag{9}$$

with $k_B = 1$, and $J = 1$, to simplify the notation. The extremum conditions can be written as

$$p = \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \varphi_2(x) \tag{10}$$

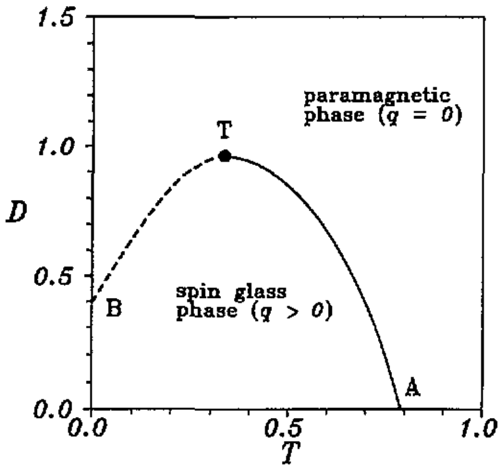


**Figure 1.** Sketch of the phase diagram as obtained by Ghatak and Sherrington in the replica-symmetric approximation. The full curve AT is the curve of second-order transitions and the broken curve BT is the suggested line of first-order transitions. Note that the first-order boundary ends at the point B where $D = 1/\sqrt{2\pi}$.

and

$$q = \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) [\varphi_1(x)]^2 \tag{11}$$

where

$$\{\varphi_1(x), \varphi_2(x)\} = \frac{2\exp\left(-x^*\sqrt{q}/T\right)}{z(x)} \left\{\sinh\left(\frac{x\sqrt{q}}{T}\right), \cosh\left(\frac{x\sqrt{q}}{T}\right)\right\}. \tag{12}$$

In figure 1 we show the $D$–$T$ phase diagram obtained by Ghatak and Sherrington from these equations. There is a spin-glass phase ($q > 0$) separated from a paramagnetic phase ($q = 0$) by a second-order transition line AT at higher temperatures, and by a first-order curve BT at lower temperatures. The paramagnetic solution has been fully analysed in the previous publications (the second-order boundary can be obtained analytically). Given $T$ and $D$, for $q = 0$, it is interesting to remark again that there may be three distinct solutions for the parameter $p$ (but only the smallest solution is stable). The tricritical point is located at $T_{\mathrm{tr}} = \frac{1}{3}$, and $D_{\mathrm{tr}} = \frac{1}{2} + \frac{1}{3}(2\ln 2) = 0.962\,098\ldots$. Although Lage and de Almeida [3] analyse the stability of the replica-symmetric solutions in the $n \to 0$ limit (and make a remark on the occurrence of complex eigenvalues of the Hessian matrix), there is no detailed study of the spin-glass phase. Ghatak and Sherrington [1] just sketch a first-order boundary and claim that it ends at $T = 0$, and $D = 1/\sqrt{2\pi}$ (which is one-half of the value suggested by Lage and de Almeida).

To perform a numerical analysis of the spin-glass phase, we have to solve the nonlinear extremum equations (10) and (11). This problem can be simplified by using the variable $x^*$, defined by (9) as an auxiliary parameter. We first solve (11) for $q$ in terms of $T$ and $x^*$. Since this is a one-variable problem, it is not difficult to see that, given $T$ and $x^*$, there is only one positive root, $q = q(T, x^*)$. Inserting this solution into (10), we determine $p = p(T, x^*)$. Both $p$ and $q$ are monotonically decreasing functions of $T$ and $x^*$. Finally, from (9), we find $D$ as a function of $T$ and $x^*$,

$$D = D\left(T, x^*\right) = \sqrt{q}x^* + \frac{p-q}{2T}. \tag{13}$$

In figure 2, we have plotted the numerical results for the spin-glass order parameter $q$ as a function of the crystal-field anisotropy $D$ at some representative temperatures. As $x^* \to -\infty$, the numerical calculations indicate that $D \to -\infty$, and $q \to q_{\mathrm{SK}}$, where $q_{\mathrm{SK}}$

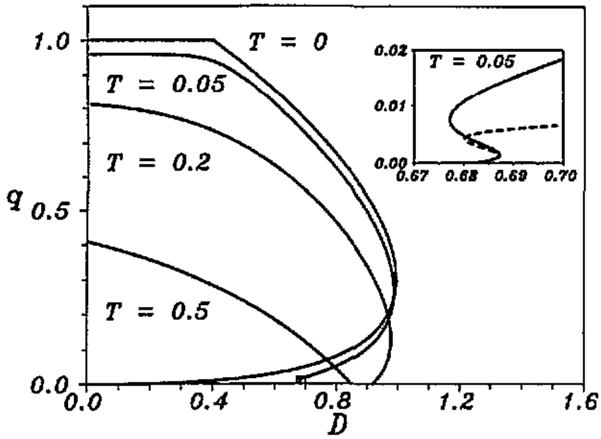


**Figure 2.** Spin-glass order parameter $q$ as a function of the anisotropy parameter $D$ for some representative temperatures. For $T > \frac{1}{3}$, the parameter $q$ is a single-valued function of $D$. For $\frac{1}{3} > T > T_0 \approx 0.058$, there is an interval of $D$ where $q$ is double valued. Finally, for $T < T_0$, there are narrow intervals of $D$ where there are three or four distinct values of $q$. The inset shows the region of small values of $q$, for $T = 0.05$; the broken curve is the asymptotic result. When there are multiple solutions, we select the largest value of $q$.

is the spin-glass order parameter of the Sherrington–Kirkpatrick model. On the other hand, as $x^* \to +\infty$, we find that $q \to 0$, and

$$D \to D_c = \tfrac{1}{2} + T \ln\left[\frac{2(1-T)}{T}\right] \tag{14}$$

which is the expression of the second-order boundary for $T > \frac{1}{3}$. All these results can be justified by asymptotic analytic calculations. The spin-glass solutions exist only up to a certain maximum value of $D$ which will be denoted $D_m$. For $T > \frac{1}{3}$, $D_m$ coincides with $D_c$ and there is only one spin-glass solution for all $D < D_m = D_c$. For $T < \frac{1}{3}$, $D_m$ is larger than $D_c$ and there are two distinct spin-glass solutions for $D_c < D < D_m$ if $T > T_0 \approx 0.058$, as illustrated for the case $T = 0.2$ in figure 2. If $T < T_0$, the situation becomes more complicated. As shown in the inset of figure 2, for $T = 0.05$, there is a narrow interval, $D_1 < D < D_2$, where there are three or four spin-glass solutions. This rather surprising result can also be confirmed by analytic asymptotic calculations.

In the presence of multiple spin-glass solutions, as in the region where there is a first-order transition, we are faced with the problem of selecting the physically meaningful result. In the paramagnetic case, we have used the stability criterion to choose the relevant solution. In the case of multiple spin-glass solutions, no such clear-cut choice is possible since none of them satisfies the stability requirements. In fact, as shown by Lage and de Almeida [3], the Hessian matrix of this problem has three distinct eigenvalues. As in the Sherrington–Kirkpatrick model, one of these eigenvalues is always negative for the replica-symmetric spin-glass solutions. The other eigenvalues, $\lambda_{\pm}$, may become negative or complex, and do not provide any clue for the selection of the spin-glass solution. However, we note that in the paramagnetic case the stable solution meets continuously with the solution at large values of $D$, where there is no ambiguity. We then follow this criterion to select the physically meaningful spin-glass solution. Namely, when there are multiple solutions, we select the branch which can be smoothly continued for small values of $D$. Indeed, this is the only consistent choice with continuous values of the free energy and the entropy

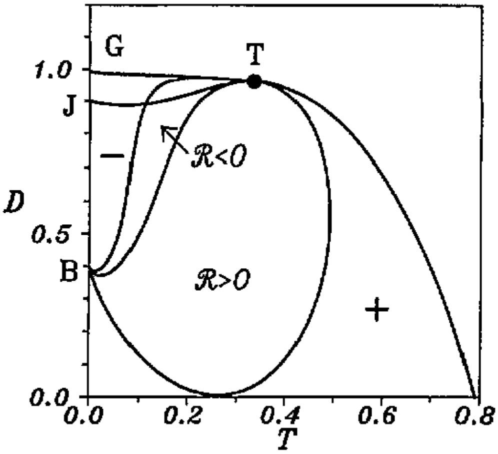


**Figure 3.** Different regions in the $D$–$T$ plane according to the nature of the eigenvalues of the Hessian matrix. In the region indicated by + (−) the eigenvalues are real and positive (negative). In the regions indicated by $\mathcal{R} > 0$ ($\mathcal{R} < 0$) the eigenvalues are complex and their real parts are positive (negative). Note that the three curves separating the different regions meet at the tricritical point T and also at the point B corresponding to $T = 0$ and $D = 1/\sqrt{2\pi}$. Also shown are the curve $D = D_m$ (curve GT) and the line of the first-order transitions (curve JT).

inside the spin-glass phase. Therefore, in the presence of multiple spin-glass solutions, we always select the largest value of the order parameter $q$. Equating the free energies of the spin-glass and the paramagnetic solutions, we locate the first-order boundary. The result is shown in figure 3, together with the regions where the eigevalues $\lambda_\pm$ are positive, negative, and complex. It is remarkable that all the stability conditions of the spin-glass solution are violated in the region where the first-order transition takes place. At $T = 0$, the first-order transition occurs at $D \approx 0.9$, which is about twice the value $1/\sqrt{2\pi}$ quoted by previous authors [1, 4].

In the $x^* \to -\infty$ limit, we have $\varphi_1(x) \to \tanh(x)$, and $\varphi_2(x) \to 1$. Therefore, the extremum conditions are given by $p \approx 1$, and

$$q \approx \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \tanh^2\left(\frac{x\sqrt{q}}{T}\right) \tag{15}$$

which is the well known expression for the Sherrington–Kirkpatrick order parameter $q_{\mathrm{SK}}$. In the opposite limit, $x^* \to +\infty$, with finite $D$, we have $q \to 0$ with $\sqrt{q}x^* < \infty$. To obtain the extremum equations, we have to evaluate integrals of the form

$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) f\left(\frac{x\sqrt{q}}{T}\right) = \frac{T}{\sqrt{q}} \int_{-\infty}^{+\infty} \frac{\mathrm{d}\xi}{\sqrt{2\pi}} \exp\left(-\frac{T^2\xi^2}{2q}\right) f(\xi)\,. \tag{16}$$

It is straightforward to expand $f(\xi)$about the origin to perform an integration term by term. We then write an expansion of $p$ in powers of $q$ and insert into (13). Finally, we have

$$D(q) = D_c + Aq + Bq^2 + Cq^3 + \cdots \tag{17}$$

where $D_c$ is given by (14), and the coefficients $A, B, C, \ldots$ are temperature-dependent. Equation (17) shows that $D(q = 0) = D_c$. The slope of the curve $D(q)$ at $q = 0$ is given by $(\partial D/\partial q)_{q=0} = A = (1 - 3T)/[2T(1 - T)]$, which is negative for $T > \frac{1}{3}$, and positive for $T < \frac{1}{3}$. As illustrated in figure 3, these results confirm the numerical calculations of the last paragraph. The surprising behaviour of the curve $D(q)$ at low temperatures is also confirmed by the asymptotic calculations, as shown by the comparison between the two results in the inset of figure 3. We can determine the approximate temperature for the onset of this kind of behaviour by requiring that the equation $\partial D/\partial q = A + 2Bq + 3Cq^2 = 0$ admits two real roots, that is, $B^2 - 3AC > 0$. The equation $B^2 - 3AC = 0$ has the solution $T_0 = 0.058\,0767\ldots$, which is in good agreement with the numerical value of $T_0$ .

where

$$t = T - \tfrac{1}{3} \tag{19}$$

$$\epsilon = D - D_{tr} - \left(\ln 4 - \tfrac{3}{2}\right)t \tag{20}$$

and

$$f_0 = \tfrac{1}{3}\left(\tfrac{1}{4} - \ln \tfrac{3}{2}\right) - \left(\tfrac{1}{4} + \ln \tfrac{3}{2}\right)t + \left(\tfrac{1}{3}\epsilon - \tfrac{3}{4}t^2\right). \tag{21}$$

*In the spin-glass phase, we choose the largest value of $q$ to obtain the free energy per spin,*

$$f_{sg} = f_0 + \tfrac{3}{4}t^3 - \tfrac{9}{4}\left(-\tfrac{8}{27}\epsilon\right)^{3/2} + O\left(t^4\right). \tag{22}$$

Equating the expressions of $f_p$ and $f_{sg}$, we obtain the asymptotic form of the first-order boundary,

$$\epsilon = -\left[\tfrac{27}{2}\cos^2\left(\tfrac{2}{9}\pi\right)\right]t^2 = -(7.922\,125\ldots)\,t^2 \tag{23}$$

with a coefficient in disagreement with the result of Mottishaw and Sherrington [4]. We have also corrected some additional results of Mottishaw and Sherrington in the neighbourhood of the tricritical point. Needless to say, our findings have always been checked against detailed numerical calculations.

To study the spin-glass solutions near $T = 0$, we have to consider the separate cases $x^* < 0$ and $x^* > 0$. For $x^* < 0$, which corresponds to $D < 1/\sqrt{2\pi}$ at $T = 0$, a straightforward analysis of the extremum conditions (10) and (11) yields the asymptotic result

$$q = 1 - \left(\frac{2}{\pi}\right)^{1/2} T - \frac{1}{\pi}T^2 + O\left(T^3\right). \tag{24}$$

Inserting into the expression of the free energy, and neglecting exponentially small contributions, we have

$$f = D - \left(\frac{2}{\pi}\right)^{1/2} + \frac{1}{2\pi}T - \frac{1}{\sqrt{2\pi}}\left(\frac{\pi^2}{12} - \frac{1}{2\pi}\right)T^2 + O\left(T^3\right). \tag{25}$$

In the more interesting case $x^* > 0$, and $T \ll 1$, the functions $\varphi_1(x)$ and $\varphi_2(x)$ are given by the asymptotic form

$$\varphi_1(x), \varphi_2(x) \approx \frac{1}{1 + \exp\left[-(\sqrt{q}/T)(x - x^*)\right]}. \tag{26}$$

Since this expression becomes a step function at $T = 0$, we can derive an asymptotic expansion for the parameter $p$, given by (10), in close analogy with the well known Sommerfeld expansion for the degenerate electron gas. Thus, we have

$$p = 1 - \sum_{n=0}^{\infty} c_{2n}\phi_{2n}\left(\frac{T}{\sqrt{q}}\right)^{2n} \tag{27}$$

where

$$c_0 = 1 \qquad c_{2n} = \frac{\left(2^{2n} - 2\right)\pi^{2n}}{2^{2n}(2n)!}|B_{2n}| \tag{28}$$

$\phi_m$ denotes the $m$th derivative of the error function evaluated at $x^*/\sqrt{2}$,

$$\phi_m = \left[\frac{d^m}{dz^m}\mathrm{erf}(z)\right]_{z=x^*/\sqrt{2}} \tag{29}$$

and $B_{2n}$ are the Bernoulli numbers [5]. The spin-glass order parameter is given by the asymptotic expression

$$q = p - \frac{T}{\sqrt{2q}} \sum_{n=0}^{\infty} c_{2n} \phi_{2n+1} \left( \frac{T}{\sqrt{q}} \right)^{2n} . \tag{30}$$

Inserting $p$, given by (27), into the equation for the free energy, we obtain

$$f \approx \frac{p^2 - q^2}{4T} - \sqrt{2q} \left[ \phi_1 - \frac{x^*}{\sqrt{2}} (1 - \phi_0) \right] - \sqrt{2q} \sum_{n=1}^{\infty} c_{2n} \phi_{2n-1} \left( \frac{T}{\sqrt{q}} \right)^{2n} . \tag{31}$$

At $T = 0$ we have

$$p\,(T = 0) = q\,(T = 0) = 1 - \phi_0 \tag{32}$$

and

$$f_{\text{sg}}\,(T = 0) = (1 - \phi_0)^{1/2} \left[ x^* (1 - \phi_0) - \frac{\sqrt{2}}{4} \phi_1 \right] \tag{33}$$

where $x^*$ as a function of $D$ comes from the equation

$$D\,(T = 0) = (1 - \phi_0)^{1/2} \left[ x^* + \frac{\sqrt{2}}{4} \frac{\phi_1}{1 - \phi_0} \right] \tag{34}$$

and $\phi_m$ is given by (29). Since the free energy of the paramagnetic phase vanishes at $T = 0$, the first-order transition is determined by the condition $f_{\text{sg}}\,(T = 0) = 0$. At the transition, we have $x^* = 0.612\,003\ldots$, from which we obtain $D = 0.899\,903\ldots$, in complete agreement with the numerical calculations, but in disagreement with the value $D = 1/\sqrt{2\pi}$ which has been quoted by previous authors [1,4]. The negative slope of the first-order boundary,

$$\left( \frac{\partial D}{\partial T} \right)_{T=0} = -\frac{1}{2\pi} \frac{\exp\left(-(x^*)^2/2\right)}{\operatorname{erfc}\left(x^*/\sqrt{2}\right)} = -0.374\,548\ldots \tag{35}$$

is related to the negative value of the ground-state entropy in the replica-symmetric approximation and also agrees with the numerical calculations.

In conclusion, we have used numerical and analytic techniques to re-analyse the replica-symmetric solutions of the spin-glass model introduced by Ghatak and Sherrington [1]. Despite the occurrence of multiple spin-glass solutions and complex eigenvalues of the Hessian matrix, it is still possible to derive a consistent physical picture at the same level of the replica-symmetric solutions of the standard Sherrington–Kirkpatrick spin-glass model [2]. In particular, we did not find a discontinuous free energy along the first-order line, as mentioned by Lage and de Almeida [3]. We rather used the continuity of the free energy to establish the correct location of the boundaries in the $D$–$T$ phase diagram. The negative slope of the first-order transition line at $T = 0$ (this slope is positive in the phase diagrams sketched by Ghatak and Sherrington [4]) is associated with the well known pathology of the ground-state entropy in the replica-symmetric approximation. Although there are no qualitative discrepancies, the asymptotic results of Mottishaw and Sherrington [4] in the vicinity of the tricritical point, in particular for the first-order line, are also slightly different from our own findings.

It should be mentioned that the replica-symmetric spin-glass solutions are always unstable and unsatisfactory. Since the instabilities are even more serious in the Ghatak–Sherrington model, it certainly poses a more stringent test for the validity the replica-symmetry-breaking schemes. In fact, we have already performed a preliminary study of this model in the first step of Parisi's replica-symmetry-breaking ansatz [6]. The solutions are in the correct direction. The zero-temperature entropy and the slope of the first-order line at $T = 0$ are less negative. We expect that, in the full Parisi solution [7] of the model, the zero-temperature entropy and the slope will be exactly zero. Finally, we wish to mention that the Ghatak and Sherrington model on a Cayley tree has been considered by da Costa and Salinas [8]. In the infinite coordination limit, the model on the tree is described by the same replica-symmetric equations of this paper and consequently leads to the same results.

## References


[1] Ghatak S K and Sherrington D 1977 *J. Phys. C: Solid State Phys.* **10** 3149

[2] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792

[3] Lage E J S and de Almeida J R L 1982 *J. Phys. C: Solid State Phys.* **15** L1187

[4] Mottishaw P and Sherrington D 1985 *J. Phys. C: Solid State Phys.* **18** 5201

[5] Abramowitz M and Stegun I 1965 *Handbook of Mathematical Functions* (New York: Dover)

[6] da Costa F A 1990 *PhD Thesis* Universidade de São Paulo

[7] Mezard M, Parisi G, and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)

[8] da Costa F A and Salinas S R 1990 *Rev. Bras. Fis.* **20** 49