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PUBLICAÇÕES

IFUSP/P-1052

FIRST-ORDER TRANSITION IN A SPIN-GLASS MODEL

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Junho/1993

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Abstract

We consider a generalization of the Sherrington-Kirkpatrick spin-glass model introduced by Ghatak and Sherrington. The model is defined for an arbitrary spin S and includes crystal field effects. For integer S, replica-symmetric calculations have shown that it can display both continuous and discontinuous transitions separated by a tricritical point. For $S = 1$, we perform a detailed analysis of the replica-symmetric solution to clarify some inconsistencies in the previous studies of the first-order transition, especially the location of the transition line in the phase diagram.

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1 Introduction

Some time has already elapsed since Parisi (Parisi 1979, 1980a, 1980b) succeeded in solving the infinite-range Sherrington-Kirkpatrick model of an Ising spin-glass (Sherrington and Kirkpatrick 1975). The model has revealed a surprising richness (Mézard *et al.* 1987), although its applicability to a three-dimensional spin-glass is still an unsettled problem (Caraccilo *et al.* 1990).

Various generalizations of the Sherrington-Kirkpatrick model have been proposed in the past (see for instance Binder and Young 1986 for a review). One such modification due to Ghatak and Sherrington (1977) generalizes the Sherrington-Kirkpatrick model to an arbitrary spin S and includes a term to account for the crystal field effects. Perhaps the most interesting aspect of this model is the possibility, for integer S, of both continuous and first-order transitions separating the paramagnetic and spin-glass phases, as shown by Ghatak and Sherrington in the replica-symmetric approximation. The stability of the replica-symmetric solution was investigated by Lage and de Almeida (1982) who also pointed out some difficulties related to the first-order transition. Mottishaw and Sherrington (1985) further investigated the model and performed Parisi's analysis along the line of continuous transitions.

Since it has been a subject of some controversy, 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 asymptotic expansions at low temperatures and close to the tricritical point. Our results for the location of the first-order line are at variance with the earlier works, but we believe this discrepancy to be due to an insufficient numerical study of the spin-glass solution by the previous authors. Although the replica-symmetric spin-glass solution is unsatisfactory, as it is everywhere unstable with respect to the replica-symmetry breaking perturbations, we believe that a correct understanding of the replica-symmetric solution is a necessary step towards more sophisticated approaches.

The layout of this paper is as follows. In Section 2 we define the general spin-S Ghatak-Sherrington model and use the replica approach to establish formal expressions for the free energy and the equation of state. In Section 3 we recover the replica-symmetric equations of Ghatak and Sherrington for a typical integer spin case, $S = 1$. Also, we give the stability conditions as obtained by Lage and de Almeida. For the sake of completeness, in Section

4 we describe the paramagnetic solutions which have already been analyzed in detail by Lage and de Almeida and Mottishaw and Sherrington. In the anisotropy (D)-temperature (T) phase diagram, there is a critical line which ends at a tricritical point. It should be remarked that, in the region of first-order transition, there may be three distinct paramagnetic solutions, although only one of them satisfies the stability requirements. The main results of this paper, given in Section 5, refer to the analysis of the spin-glass solutions. In Section 5.1 we report detailed numerical calculations to show that, in the region $D > 0$ of the $D - T$ phase diagram, there may be up to four distinct spin-glass solutions. Unlike the paramagnetic case, these spin-glass solutions are all unstable. As in the Sherrington-Kirkpatrick model, there is always a negative eigenvalue of the Hessian matrix. The other eigenvalues, however, may be negative or even complex in large regions of the phase diagram. Since the stability requirements are of no help for the selection of the valid spin-glass solution we choose the branch that meets continuously with the spin-glass solution for $D < 0$, where there is no ambiguity. Equating the free energies of the paramagnetic and the spin-glass solutions, we obtain the first-order boundary. It is remarkable that in this region all the stability conditions are violated. In Sections 5.2 - 5.4, we perform detailed asymptotic calculations to confirm the numerical findings. The vicinity of the tricritical point had already been analyzed by Mottishaw and Sherrington. Although getting the same asymptotic paramagnetic and spin-glass solutions, we obtain different numerical coefficients for the asymptotic expression of the first-order boundary. The numerical calculations, however, support our asymptotic results. In Section 5.4, we use the well known Sommerfeld expansion to obtain asymptotic results near zero temperature. In complete agreement with the numerical calculations, the first-order transition for $T = 0$ is located at $D = 0.89903306\ldots$, far from the value $1/\sqrt{2\pi}$ quoted by the previous authors. The zero-temperature entropy is always negative for the spin-glass solution, as expected considering the replica-symmetric nature of our calculations. Finally, some conclusions are presented in Section 6.

2 The model and basic equations

The infinite-range spin-glass model introduced by Ghatak and Sherrington (1977) is given by the Hamiltonian

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

where the N spins S_i can take the values $0, \pm 1, \ldots, \pm S$; the (ij) sum is over all distinct pairs of spins; the exchange interactions J_{ij} are quenched, independent random variables with the Gaussian distribution

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

and D is the crystal field anisotropy parameter. For $S = 1$, in the limit $D \to -\infty$ we regain the Sherrington-Kirkpatrick model of an Ising spin-glass.

In the replica approach the identity $\ln x = \lim_{n\to 0}[(x^n - 1)/n]$ is used to recast the free energy per spin f in the form

$$-\frac{f}{kT} = \lim_{N\to\infty} \frac{1}{N} \overline{\ln Z} = \lim_{N\to\infty} \lim_{n\to 0} \frac{1}{Nn}(\overline{Z^n} - 1), \tag{3}$$

where the bar denotes configurational average and T is the absolute temperature. Evaluating $\overline{Z^n}$ for integer n and taking the thermodynamic limit, $N \to \infty$, before the $n \to 0$ limit, we obtain (Lage and de Almeida 1982, Mottishaw and Sherrington 1985),

$$f = \lim_{n\to 0} \frac{1}{n} \{\min_{p_\alpha, q_{\alpha\beta}} f_n[p_\alpha, q_{\alpha\beta}]\}, \tag{4}$$

where

$$f_n[p_\alpha, q_{\alpha\beta}] = \frac{J^2}{4kT}\sum_\alpha p_\alpha^2 + \frac{J^2}{2kT}\sum_{(\alpha\beta)} q_{\alpha\beta}^2 - kT \ln Z_n[p_\alpha, q_{\alpha\beta}], \tag{5}$$

$$Z_n[p_\alpha, q_{\alpha\beta}] = \mathrm{Tr}_{\{S^\alpha\}} \exp\{\mathcal{H}_n[p_\alpha, q_{\alpha\beta}]\}, \tag{6}$$

$$\mathcal{H}_n[p_\alpha, q_{\alpha\beta}] = (\frac{J}{kT})^2 \sum_{(\alpha\beta)} q_{\alpha\beta} S^\alpha S^\beta + \frac{1}{2}(\frac{J}{kT})^2 \sum_\alpha p_\alpha (S^\alpha)^2 - \frac{D}{kT}\sum_\alpha (S^\alpha)^2. \tag{7}$$

The indices α and β run from 1 to n and (α, β) denotes distinct pairs with $\alpha \neq \beta$.

The condition for $f_n[p_\alpha, q_{\alpha\beta}]$ to be an extremum is given by the equations

$$p_\alpha = \langle (S^\alpha)^2 \rangle, \qquad q_{\alpha\beta} = \langle S^\alpha S^\beta \rangle, \tag{8}$$

where $\langle \ldots \rangle$ denotes the thermal average with respect to the replica hamiltonian (7). The internal energy per spin follows from the thermodynamic relation $u = f - T\partial f/\partial T$, and equations (4) and (8),

$$u = \lim_{n\to 0} \frac{1}{n}\left[D\sum_\alpha p_\alpha - \frac{J^2}{kT}\sum_{(\alpha\beta)} q^2_{\alpha\beta} - \frac{J^2}{2kT}\sum_\alpha p^2_\alpha\right]. \tag{9}$$

3 The replica-symmetric solution

In the rest of this paper we will restrict to the case of spin $S = 1$. We will also set $k = 1$ and $J = 1$ throughout. Within the replica-symmetric *Ansatz* we look for solutions of the extremum equations (8) of the form

$$p_\alpha = p \quad \text{and} \quad q_{\alpha\beta} = q \tag{10}$$

for all α and β. We then find free energy per spin,

$$f = \frac{p^2 - q^2}{4T} - T\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \ln z(x), \tag{11}$$

where

$$z(x) = 1 + 2\, e^{-\sqrt{q}x^*/T} \cosh\left(\frac{\sqrt{q}}{T}x\right), \tag{12}$$

$$x^* = \frac{1}{\sqrt{q}}\left(D - \frac{p-q}{2T}\right). \tag{13}$$

The extremum equations (8) can be written as

$$p = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \varphi_2(x), \tag{14}$$

$$q = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} [\varphi_1(x)]^2. \tag{15}$$

where

$$\varphi_1(x) = \frac{2e^{-\sqrt{q}x^*/T}}{z(x)} \sinh\left(\frac{\sqrt{q}}{T}x\right), \tag{16}$$

$$\varphi_2(x) = \frac{2e^{-\sqrt{q}x^*/T}}{z(x)} \cosh\left(\frac{\sqrt{q}}{T}x\right). \tag{17}$$

The internal energy per spin (9) becomes

$$u = Dp - \frac{p^2 - q^2}{2T}. \tag{18}$$

These equations were derived by Ghatak and Sherrington (1977), who also studied various other thermodynamic quantities. The sketch of their phase diagram is reproduced in figure 1. We observe the existence of a spin glass phase ($q > 0$) separated from the paramagnetic phase ($q = 0$) by a second-order transition line AT at higher temperatures and by a first-order transition line BT at lower temperatures. In their work, Ghatak and Sherrington do not mention the exact location of the tricritical point T nor the exact expression for the second-order line AT. However they claim that the first-order line ends for $T = 0$ at the point B where $D = 1/\sqrt{2\pi}$, a result which does not agree with our calculations.

The stability analysis of the replica-symmetric solution was performed by Lage and de Almeida (1982). In the limit $n \to 0$ there are only three distinct eigenvalues of the Hessian matrix given by

$$\begin{aligned}\lambda_\pm &= \frac{1}{2}[(A-B)+(P-4Q+3R)] \pm \\ &\pm\frac{1}{2}\sqrt{[(A-B)-(P-4Q+3R)]^2-8(C-D)^2}, \qquad (19)\\ \lambda &= P-2Q+R, \qquad (20)\end{aligned}$$

where

$$\begin{aligned}A-B &= 2T^2 - \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}e^{-x^2/2}\varphi_2(x)[1-\varphi_2(x)], \qquad (21)\\ C-D &= \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}e^{-x^2/2}\varphi_1(x)^2[\varphi_2(x)-1], \qquad (22)\\ P-4Q+3R &= T^2-\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}e^{-x^2/2}[\varphi_2(x)^2+3\varphi_1(x)^4 - \\ &\quad -4\varphi_1(x)^2\varphi_2(x)], \qquad (23)\\ P-2Q+R &= T^2-\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}}e^{-x^2/2}[\varphi_2(x)-\varphi_1(x)^2]^2. \qquad (24)\end{aligned}$$

The local stability requires all three eigenvalues to be non-negative.

4 The paramagnetic solution

The paramagnetic solution ($q = 0$) has been analyzed in considerable detail by Lage and de Almeida (1982) and by Mottishaw and Sherrington (1985).

We merely summarize their findings for the sake of completeness.

Equation (14) for the order parameter p reduces for $q = 0$ to

$$p = \left(1+\frac{1}{2}e^{D/T-p/2T^2}\right)^{-1}. \qquad (25)$$

This equation admits three distinct solutions for $D_- < D < D_+$, where

$$D_\pm = \left(\frac{1\pm\sqrt{1-8T^2}}{4T}\right) - 2T\ln\left(\frac{1\pm\sqrt{1-8T^2}}{4T}\right), \qquad (26)$$

and a single solution otherwise [Mottishaw and Sherrington (1985)].

The conditions for the eigenvalues (19)-(20) to be non-negative reduce in this case simply to

$$p < \begin{cases}\frac{1-\sqrt{1-8T^2}}{2} & \text{for } T<\frac{1}{3}\\ T & \text{for } T>\frac{1}{3}\end{cases} \qquad (27)$$

which implies that there are no stable paramagnetic solutions if [Lage and de Almeida (1982)]

$$D < \begin{cases}D_- & \text{for } T<1/3\\ D_c & \text{for } T>1/3\end{cases} \qquad (28)$$

where

$$D_c = \frac{1}{2}+T\ln\left[\frac{2(1-T)}{T}\right]. \qquad (29)$$

The curves $D = D_c$ and $D = D_\pm$ are shown in figure 2. The curve $D = D_c$ corresponds to the second-order transition line AT and the curve $D = D_-$ to the line DE. According to equation (28) there are no stable paramagnetic solutions below the curve ATE. The location of the tricritical point T is given by

$$\left.\begin{aligned} T_{tr} &= \tfrac{1}{3} \\ D_{tr} &= \tfrac{1}{2} + \tfrac{2}{3}\ln 2 = 0.962098\ldots \end{aligned}\right\} \tag{30}$$

We observe that in the region where the first-order transition takes place equation (25) admits three distinct solutions, as shown in figure 3. However only the *smallest* solution satisfies the stability condition.

The free energy per spin (11) of the paramagnetic solution is given by

$$f_{\mathrm{P}} = \frac{p^2}{4T} + T\ln(1-p). \tag{31}$$

The smallest solution of equation (25) at low temperatures is given asymptotically for $D > 0$ by

$$p \approx 2e^{-D/T}. \tag{32}$$

Therefore the free energy per spin (11) at low temperatures is given asymptotically by

$$f_{\mathrm{P}} \approx \frac{e^{-2D/T}}{T}. \tag{33}$$

At the absolute zero of temperature the free energy of the paramagnetic solution is identically zero, irrespective of $D > 0$.

5 The spin-glass solution

5.1 Numerical results

The main numerical problem is the solution of the extremum equations (14) and (15) for p and q. The difficulty, common to the solution of all systems of nonlinear equations, is the possibility of missing some relevant solutions due, for example, to a poorly chosen initial guess. In this case, however, it is possible to find all the solutions by using the variable x^* defined in equation (13) as an auxiliary parameter. We first solve equation (15) for q in terms of T and x^*, and since this is a one variable problem it is not difficult to ascertain numerically that there is only one positive root for given T and x^*,

$$q = q(T, x^*). \tag{34}$$

Substituting this solution for q into equation (14) we determine p,

$$p = p(T, x^*). \tag{35}$$

Both q and p are monotonically decreasing functions of x^*. Finally, from equation (13) we find D as a function of T and x^*,

$$D = D(T, x^*) = \sqrt{q}x^* + \frac{p-q}{2T}. \tag{36}$$

In figure 4 we have plotted the numerical results for the spin glass order parameter q as a function of the crystal field anisotropy D for some representative temperatures. Numerically we found that as $x^* \to -\infty$, $D \to -\infty$ and $q \to q_{SK}$, where q_{SK} is the spin-glass order parameter of the Sherrington-Kirkpatrick model. On the other hand as $x^* \to \infty$ we found that $D \to D_c$, where D_c is given by equation (29), and $q \to 0$. These results will be given analytical justification in the asymptotic calculations discussed in the next subsection. The spin-glass solutions exist only up to a certain maximum value of D, which will be denoted D_m. For $T > 1/3$, D_m coincides with D_c and there is only one spin-glass solution $q > 0$ for all $D < D_m = D_c$. For $T < 1/3$, D_m is larger that 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 4. If $T < T_0$ the situation becomes more complicated. As shown in the inset of figure 4, for $T = 0.05$ there is a very narrow interval $D_1 < D < D_2$ where there are three or four distinct spin-glass solutions. This rather surprising result is nevertheless confirmed by analytical calculations to be discussed in the next subsection. Figure 5 shows the curves D_c, D_m, D_1 and D_2 which delimit in the $D-T$ plane the regions where different numbers of spin-glass solutions are possible.

The graphs of the free energy per spin (11) of the spin-glass solution as a function of D for different temperatures are shown in figure 6. Larger values of the free energy correspond to smaller values of q. The entropy per spin given by the thermodynamic relation $s = (u - f)/T$ can be computed with the aid of expressions (11) and (18). Figure 7 shows the entropy per spin as a function of D for different temperatures. We observe that the entropy may become negative at low temperatures just as in the Sherrington-Kirkpatrick model in the replica-symmetric approximation.

When there are multiple spin-glass solutions, which is the case in the region where the first-order transition takes place, we are faced with the problem of selecting the appropriate solution. We recall that in the case of multiple paramagnetic solutions we picked up the solution which met all the stability conditions. In the case of multiple spin-glass solutions no such clear-cut choice is possible since none of them will satisfy all the stability conditions. In fact, the eigenvalue λ given by equation (20) is negative for all spin-glass solutions, just as in the Sherrington-Kirkpatrick model. However, contrary to the Sherrington-Kirkpatrick model, the eigenvalues $\lambda_\pm$ given by (19) may become negative or complex [Lage and de Almeida (1982), Mottishaw and Sherrington (1985)]. In figures 8 and 9 we have plotted the eigenvalues $\lambda_\pm$ as a function of D for $T = 0.45$ and $T = 0.08$, respectively. These graphs show the real part of $\lambda_\pm$ when they are complex. For $T > 1/3$ the eigenvalues $\lambda_\pm$ as well as their real part are always positive. For $T < 1/3$, however, the eigenvalues $\lambda_\pm$ and their real part may become negative for large values of D. In figure 9 eigenvalues $\lambda_\pm$ are double valued in the interval $D_c < D < D_m$ corresponding to the two distinct spin-glass solutions.

The numerical study of the eigenvalues of the stability matrix shows that, contrary to the paramagnetic case, they provide no clue for the selection of the spin-glass solution. On the other hand, we notice that in the paramagnetic case the stable solution meets continuously with the solution at large D values, where there is only one solution. We believe that this indicates a criterion to select the appropriate spin-glass solution, namely, when there are multiple solutions the valid spin-glass solution should meet continuously with the solution for small D values, where there is no ambiguity. Indeed, this is the only consistent choice with a continuous free energy and entropy inside the spin-glass phase as it is evident from the graphs in the figures 6 and 7. Therefore, when there are multiple spin-glass solutions, we select that one with the *largest* spin-glass order parameter q.

Equating the free energies of the spin-glass and paramagnetic solutions we locate the first-order transition. The result is depicted in figure 10 together with the regions where the eigenvalues $\lambda_\pm$ are positive, negative or complex. It is remarkable that in the region where the first-order transition takes place all the stability conditions of the spin-glass solution are violated. The first-order transition at $T = 0$ occurs at $D \approx 0.9$, which is more than twice the value $1/\sqrt{2\pi}$ quoted by the previous authors. This and other results of the numerical calculations will be confirmed by analytical calculations at low temperatures to be developed in subsection 5.4.

5.2 Asymptotic results for $x^* \to \pm\infty$

In this subsection we obtain asymptotic solutions of the extremum equations (14) and (15) for $x^* \to \pm\infty$. The main purpose of these calculations is to check the numerical results of the previous subsection.

In the limit $x^* \to -\infty$ equations (12), (16) and (17) show that we have in leading order $\varphi_1(x) \approx \tanh(x)$ and $\varphi_2(x) \approx 1$. Therefore the extremum equations (14) and (15) become

$$p \approx 1, \tag{37}$$

$$q \approx \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \tanh^2\left(\frac{\sqrt{q}}{T}x\right). \tag{38}$$

We recognize equation (38) as the expression for the Sherrington-Kirkpatrick order parameter q_{SK}. This result is to be expected since from equation (36) we have $D \to -\infty$ for $x^* \to -\infty$.

In the opposite limit, $x^* \to \infty$, if we demand D to be finite, equation (36) implies that $q \to 0$ in such a way that $\sqrt{q}x^* < \infty$. The extremum equations (14) and (15) require the evaluation of integrals of the form

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} f(\frac{\sqrt{q}}{T}x) = \frac{T}{\sqrt{q}} \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi}} e^{-T^2\xi^2/2q} f(\xi), \tag{39}$$

for $q \to 0$. Clearly the main contribution to the integral comes from the neighborhood of the origin. Thus, expanding $f(\xi)$ around the origin and integrating term by term we obtain

$$\int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} f(\frac{\sqrt{q}}{T}x) = \sum_{n=0}^{\infty} \frac{1}{2^n n!} \left(\frac{\sqrt{q}}{T}\right)^{2n} f^{(2n)}(0). \tag{40}$$

Using this result we can expand the extremum equations (14) and (15) in the forms

$$p = a + \frac{a(1-a)}{2T^2}q + \frac{a(1-7a+6a^2)}{8T^4}q^2 + \frac{a(1-31a+120a^2-90a^3)}{48T^6}q^3 + \ldots, \tag{41}$$

and

$$q = \frac{a^2}{T^2}q + \frac{a^2(1-3a)}{T^4}q^2 + \frac{a^2(8-75a+135a^2)}{12T^6}q^3 + \frac{a^2(8-189a+945a^2-1260a^3)}{24T^8}q^4 + \ldots, \tag{42}$$

where

$$a = \left(1 + \frac{1}{2}e^{\sqrt{q}x^*/T}\right)^{-1}. \tag{43}$$

From equation (42) we find

$$a = T + \left(\frac{3T-1}{2T}\right)q + \left(\frac{3T+1}{24T^3}\right)q^2 + \left(\frac{126T^3-90T^2+9T+1}{48T^5}\right)q^3 + \ldots, \tag{44}$$

and substituting into equation (41) we obtain

$$p = T + q - \left(\frac{9T^2-6T+1}{12T^3}\right)q^2 + \left(\frac{6T^2-5T+1}{2T^4}\right)q^3 + \ldots, \tag{45}$$

Finally, inserting (44) and (45) into equation (36) we obtain D as a function of q correct to order q^3,

$$D(q) = D_c + Aq + Bq^2 + Cq^3 + \ldots, \tag{46}$$

where D_c is given by equation (29) and

$$A = \frac{1-3T}{2T(1-T)}, \tag{47}$$

$$B = -\frac{1-10T+48T^2-90T^3+63T^4}{24T^4(1-T)^2}, \tag{48}$$

$$C = \frac{3-31T+129T^2-255T^3+240T^4-90T^5}{12T^5(1-T)^3}. \tag{49}$$

Equation (46) shows that $D(q=0) = D_c$. The slope of the curve $D(q)$ at $q=0$ is given by $(\partial D/\partial q)_{q=0} = A$, which is negative for $T > 1/3$ and positive for $T < 1/3$. These results confirm the numerical calculations of the previous subsection as illustrated by figure 4. The surprising behavior 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 4. We can determine the approximate temperature at which this behavior begins 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 $T_0 = 0.0580767\ldots$ which is in good agreement with the value of T_0 found numerically.

5.3 Asymptotic results near the tricritical point

The behavior of the replica-symmetric solution in the vicinity of the tricritical point has been studied in considerable detail by Mottishaw and Sherrington

(1985). However, as many of their conclusions seem to be in disagreement with our numerical results, we decided to repeat their calculations.

Following Mottishaw and Sherrington we define

$$t = T - 1/3, \tag{50}$$

$$\varepsilon = D - D_{tr} - (\ln 4 - 3/2)t, \tag{51}$$

$$r = p - 1/3, \tag{52}$$

which, together with the spin-glass order parameter q, serve as expansion parameters in the vicinity of the tricritical point (30). The line $\varepsilon = 0$ is tangent to the second order curve (29) at the tricritical point. We will assume in the following that in the region of interest $r, q = O(t)$ and $\varepsilon = O(t^2)$.

Applying the expansion (40), valid for small q, to the integral in the expression of the free energy (11) we obtain

$$\begin{aligned} f &= D - T\ln 2 + \frac{p^2 - q^2}{4T} - \frac{p-q}{2T} + T\ln a - \left(\frac{a}{2T}\right) q - \\ &\quad - \frac{a(1-3a)}{8T^3} q^2 - \frac{a(1-15a+30a^2)}{48T^5} q^3 - \ldots, \end{aligned} \tag{53}$$

where a is given by equation (43). Using (50)- (52) and keeping up to third order terms we find

$$\begin{aligned} f &= f_0 + \frac{1}{8}\left(18t^3 - 36rt^2 + 36r^2t - 3r^3 - 36q^2t + \right. \\ &\quad \left. +36q^2r - 24q^3 + 8\varepsilon r\right) + O(t^4), \end{aligned} \tag{54}$$

where

$$f_0 = \frac{1}{3}\left(\frac{1}{4} - \ln\frac{3}{2}\right) - \left(\frac{1}{4} + \ln\frac{3}{2}\right)t + \left(\frac{\varepsilon}{3} - \frac{3}{4}t^2\right). \tag{55}$$

The conditions for f to be an extremum with respect to q and r are given by

$$\frac{\partial f}{\partial q} = -9q(q + t - r) = 0, \tag{56}$$

$$\frac{\partial f}{\partial r} = \varepsilon + \frac{9}{8}\left(4q^2 - r^2 + 8rt - 4t^2\right) = 0. \tag{57}$$

Equation (56) admits the solutions

$$q = 0 \quad \text{and} \quad q = r - t, \tag{58}$$

corresponding, respectively, to the paramagnetic and spin-glass solutions.

Inserting the paramagnetic solution $q = 0$ into equation (57) and solving the resulting quadratic equation in r we find two roots, $r = 4t \pm \sqrt{12t^2 + \frac{8}{9}\varepsilon}$. According to the stability analysis of section 4, the stable paramagnetic solution corresponds to the smallest value of p. Therefore the stable solution is given by

$$r = 4t - \sqrt{12t^2 + \frac{8}{9}\varepsilon}. \tag{59}$$

This result is in agreement with Mottishaw and Sherrington . Substituting $q = 0$ and r given by (59) in (54) we obtain the paramagnetic free energy per spin

$$f_p = f_0 + \frac{129}{4}t^3 + 4\varepsilon t - \frac{3}{2}\left(12t^2 + \frac{8}{9}\varepsilon\right)^{\frac{3}{2}} + O(t^4). \tag{60}$$

On the other hand, substituting the spin-glass solution $q = r - t$ into equation (57), we find the roots $r = \pm(-8\varepsilon/27)^{1/2}$. Following the discussion of subsection 5.1 we choose the value of r corresponding to the largest spin-glass order parameter q, that is,

$$r = \left(-\frac{8}{27}\varepsilon\right)^{1/2}, \tag{61}$$

$$q = \left(-\frac{8}{27}\varepsilon\right)^{1/2} - t, \qquad (62)$$

in agreement with Mottishaw and Sherrington . Inserting (61) and (62) in (54) we obtain the spin-glass free energy per spin,

$$f_{sg} = f_0 + \frac{3}{4}t^3 - \frac{9}{4}\left(-\frac{8}{27}\varepsilon\right)^{3/2} + O(t^4). \qquad (63)$$

Equating the free energies (60) and (63) we find the asymptotic form of the first-order transition line

$$\varepsilon = -\left[\frac{27}{2}\cos^2\left(\frac{2\pi}{9}\right)\right]t^2 = -(7.922125\ldots)t^2. \qquad (64)$$

This result is in disagreement with the result of Mottishaw and Sherrington who found for the coefficient of t^2 the value -12.15 instead of $-7.922125\ldots$.

Other asymptotic results obtained by Mottishaw and Sherrington relate to the nature of the eigenvalues $\lambda_\pm$ given in (19). The condition for these eigenvalues to be real is

$$\Delta = \Delta_+\Delta_- > 0, \qquad (65)$$

where

$$\Delta_\pm = (A-B) - (P - 4Q + 3R) \pm 2\sqrt{2}(C-D). \qquad (66)$$

When the eigenvalues $\lambda_\pm$ are complex, their real part is given by

$$\mathcal{R} = \frac{1}{2}[(A-B) + (P - 4Q + 3R)]. \qquad (67)$$

Applying the expansion (40) to the various integrals in equations (21)-(24), and using (50)-(52) we obtain

$$\Delta_\pm = \frac{2}{3}t + \frac{1}{3}r - \frac{4}{3}(1 \pm \sqrt{2})q + O(t^2), \qquad (68)$$

$$\mathcal{R} = t - \frac{1}{2}r + \frac{2}{3}q + O(t^2). \qquad (69)$$

Substitution of the spin-glass solutions (61) and (62) gives

$$\Delta_\pm = \left(2 \pm \frac{4\sqrt{2}}{3}\right)t - \left(1 \pm \frac{4\sqrt{2}}{3}\right)\left(-\frac{8}{27}\varepsilon\right) + O(t^2), \qquad (70)$$

$$\mathcal{R} = t - \frac{1}{3}t + \frac{1}{6}\left(-\frac{8}{27}\varepsilon\right) + O(t^2). \qquad (71)$$

Above the tricritical temperature, $t > 0$, Δ_+ vanishes along the line

$$\varepsilon = -\frac{27}{1058}(84\sqrt{2} + 121)t^2 = -(6.119505\ldots)t^2, \qquad (72)$$

whereas below the tricritical temperature, $t < 0$, Δ_- vanishes along the line

$$\varepsilon = -\frac{27}{1058}(84\sqrt{2} - 121)t^2 = -(0.056298\ldots)t^2. \qquad (73)$$

These results are also in disagreement with Mottishaw and Sherrington who found -4.446 instead of $-6.119505\ldots$ and -0.2971 instead of $-0.056298\ldots$. Below the tricritical temperature $\mathcal{R}$ vanishes along the line

$$\varepsilon = -\frac{27}{2}t^2 = -13.5\, t^2, \qquad (74)$$

which separates regions with differing signs of the real part of $\lambda_\pm$.

Finally, let us consider the asymptotic behavior of the line D_m above which there are no spin-glass solutions. From Figure 4 it is clear that this line is determined by the condition $\partial q/\partial D = \infty$. Using the asymptotic spin-glass solution (62) we find the result $\varepsilon = 0$. Therefore, close to the tricritical point, the curves D_m and D_c coincide to order t^2.

Figure 11 shows the various curves computed numerically in the vicinity of the tricritical point. These numerical results, obtained quite independently from the asymptotic calculations of this subsection, are in agreement with our results and are incompatible with those obtained by Mottishaw and Sherrington .

5.4 Asymptotic results at low temperatures

To study the behavior of the spin-glass solution near the absolute zero of temperature we have to distinguish the cases $x^* < 0$ and $x^* > 0$. For $x^* < 0$, we write equations (14)-(15) for p and q in the form

$$p = 1 - \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2}[1 - \varphi_2(x)], \tag{75}$$

$$q = 1 - \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2}[1 - \varphi_1(x)^2]. \tag{76}$$

Since $1 - \varphi_2(x) = O(e^{\sqrt{q}x^*/T})$ the integral in equation (75) makes only an exponentially negligible contribution, and we have

$$p \approx 1. \tag{77}$$

On the other hand the function $1 - \varphi_1(x)^2$ is sharply peaked at the origin. Using this fact we obtain the asymptotic expansion

$$q \approx 1 - \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{T}{\sqrt{q}}\right) \sum_{n=o}^{\infty} (-1)^n b_{2n} \left(\frac{T}{\sqrt{q}}\right)^{2n}, \tag{78}$$

where we have neglected exponentially small terms and the coefficients b_{2n} are given by

$$b_0 = 1, \quad b_{2n} = \frac{(2^{2n} - 2)\pi^{2n}}{2^{3n} n!} \mid B_{2n} \mid, \tag{79}$$

where B_{2n} are the Bernouilli numbers (Abramowitz and Stegun 1965). The result (78) is identical to the low temperature expansion of the spin-glass order parameter in the Sherrington-Kirkpatrick model. We conclude that at low temperatures the two models behave similarly if $x^* < 0$, which corresponds, at $T = 0$, to $D < 1/\sqrt{2\pi}$. These facts have already been observed by Ghatak and Sherrington (1977). From equation (78) we obtain

$$q = 1 - \left(\frac{2}{\pi}\right)^{1/2} T - \frac{1}{\pi} T^2 + O(T^3). \tag{80}$$

Neglecting exponentially small contributions, the free energy (11) for the case $x^* < 0$ becomes

$$f \approx D - \frac{(1-q)^2}{4T} - T \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \ln\left[2\cosh\left(\frac{\sqrt{q}}{T} x\right)\right]. \tag{81}$$

Except for the additive term D, this expression is identical to the free energy of the Sherrington-Kirkpatrick model. Observing that

$$\frac{\partial}{\partial T} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-x^2/2} \ln\left[2\cosh\left(\frac{\sqrt{q}}{T} x\right)\right] = -\frac{q(1-q)}{T^3}, \tag{82}$$

and using equation (78) a term by term integration gives the following low temperature expansion of the free energy,

$$f \approx D - \frac{(1-q)^2}{4T} - \sqrt{q}\left(\frac{2}{\pi}\right)^{1/2} \left[1 + \sum_{n=1}^{\infty} \frac{(-1)^{n-1} b_{2n}}{2n-1} \left(\frac{T}{\sqrt{q}}\right)^{2n}\right]. \tag{83}$$

Substituting (80) in (83) we find

$$f \approx D - \left(\frac{2}{\pi}\right)^{1/2} + \frac{T}{2\pi} - \frac{1}{\sqrt{2\pi}} \left(\frac{\pi^2}{12} - \frac{1}{2\pi}\right) T^2 + O(T^3). \tag{84}$$

For $x^* > 0$ the functions $\varphi_1(x)$ and $\varphi_2(x)$ defined in equations (14) and (15) may be approximated by

$$\left.\begin{array}{l} \varphi_1(x) \\ \varphi_2(x) \end{array}\right\} \approx \frac{1}{1 + e^{-\sqrt{q}(x - x^*)/T}}, \tag{85}$$

where exponentially small terms have been neglected. For $T = 0$ the function (85) is a step function, and for $T << 1$ we can derive an asymptotic expansion for the order parameter p given by equation (14) in close analogy with the Sommerfeld expansion for the degenerate electron gas. Thus we find

$$p = 1 - \sum_{n=0}^{\infty} c_{2n}\phi_{2n}\left(\frac{T}{\sqrt{q}}\right)^{2n}, \tag{86}$$

where

$$c_0 = 1, \quad c_{2n} = \frac{(2^{2n}-2)\pi^{2n}}{2^n(2n)!} \mid B_{2n} \mid, \tag{87}$$

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

$$\phi_m = \left[\frac{d^m}{dz^m}\mathrm{erf}(z)\right]_{z=x^*/\sqrt{2}}. \tag{88}$$

The asymptotic expansion for the spin-glass order parameter q can be obtained most easily using the relation

$$q - p \approx \frac{T}{\sqrt{q}}\frac{\partial}{\partial x^*}p, \tag{89}$$

valid except for exponentially small terms. This result follows from the definitions of p and q given by (14) and (15), and the approximation (85). Hence,

$$q - p \approx -\left(\frac{T}{\sqrt{q}}\right)\frac{1}{\sqrt{2}}\sum_{n=0}^{\infty} c_{2n}\phi_{2n+1}\left(\frac{T}{\sqrt{q}}\right)^{2n}. \tag{90}$$

Similarly, the asymptotic expansion for the free energy can be obtained by observing that equation (11) can be written as

$$f = \frac{p^2 - q^2}{4T} - \sqrt{q}\int_{x^*}^{\infty} p(x^*)dx^*. \tag{91}$$

Inserting p given by equation (86) into equation (91) we obtain

$$f \approx \frac{p^2 - q^2}{4T} - \sqrt{2q}\left[\phi_1 - \frac{x^*}{\sqrt{2}}(1-\phi_0)\right] - \sqrt{2q}\sum_{n=1}^{\infty} c_{2n}\phi_{2n-1}\left(\frac{T}{\sqrt{q}}\right)^{2n}. \tag{92}$$

The order parameter p and q are equal at $T = 0$ and given by

$$p(T=0) = q(T=0) = 1 - \phi_0 = \mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right), \tag{93}$$

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

$$\begin{aligned} D(T=0) &= (1-\phi_0)^{1/2}\left(x^* + \frac{\sqrt{2}}{4}\frac{\phi_1}{1-\phi_0}\right) = \\ &= [\mathrm{erfc}(\frac{x^*}{\sqrt{2}})]^{1/2}\left[x^* + \frac{1}{\sqrt{2\pi}}\frac{e^{-x^{*2}/2}}{\mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right)}\right]. \end{aligned} \tag{94}$$

We observe that $D(x^* = 0) = 1/\sqrt{2\pi}$ and $D(x^* \to +\infty) = 0$. Figure 12 shows the order parameter p and q as a function of D for $T = 0$.

The free energy at the absolute zero of temperature is found to be

$$\begin{aligned} f_{sg}(T=0) &= (1-\phi_0)^{1/2}\left[x^*(1-\phi_0) - \frac{\sqrt{2}}{4}\phi_1\right] = \\ &= [\mathrm{erfc}(\frac{x^*}{\sqrt{2}})]^{1/2}\left[x^*\mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right) - \frac{1}{\sqrt{2\pi}}e^{-x^{*2}/2}\right], \end{aligned} \tag{95}$$

where x^* as a function of D is given by equation (84). The free energy (95) as a function of D has been plotted in figure 13. Since by equation (33) the free energy of the paramagnetic solution at $T = 0$ is equal to zero, the first-order transition at the absolute zero is found by setting $f_{sg}(T = 0) = 0$, which gives

$$x^*\mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right) = \frac{1}{\sqrt{2\pi}}e^{-x^{*2}/2}. \tag{96}$$

A numerical solution of this equation gives

$$x^* = 0.6120031809\ldots \tag{97}$$

From equation (95) we obtain,

$$D_{\mathrm{p-sg}}(T=0) = 0.8999033063\ldots, \tag{98}$$

which is to be compared with the value $1/\sqrt{2\pi} = 0.398942\ldots$ quoted by the previous works for the location of the transition at $T = 0$. The low temperature behavior of the entropy can be derived using the thermodynamic relation $s = (u-f)/T$ and equations (11) and (18). For the zero temperature entropy in the spin-glass phase we find

$$s_{\mathrm{sg}}(T=0) = -\frac{\phi_1^2}{8(1-\phi_0)} = -\frac{e^{-x^{*2}}}{2\pi\mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right)}, \tag{99}$$

where x^* as a function of D is given by equation (94). The zero temperature entropy is depicted in figure 14. Notice that the entropy is always negative and equal to the value of the zero temperature entropy of the Sherrington-Kirkpatrick model $-1/2\pi$ for $D < 1/\sqrt{2\pi}$.

The slope of the first-order transition line at $T = 0$ can be obtained from the Clausius-Clapeyron equation,

$$\left(\frac{\partial D}{\partial T}\right)_{T=0} = \left(\frac{s_{\mathrm{sg}} - s_{\mathrm{p}}}{p_{\mathrm{sg}} - p_{\mathrm{p}}}\right)_{T=0}. \tag{100}$$

Since $s_{\mathrm{p}} = 0$ and $p_{\mathrm{p}} = 0$, we find

$$\left(\frac{\partial D}{\partial T}\right)_{T=0} = -\frac{1}{2\pi}\left[\frac{e^{-x^{*2}/2}}{\mathrm{erfc}\left(\frac{x^*}{\sqrt{2}}\right)}\right] = -0.374548\ldots. \tag{101}$$

This result is in agreement with the first-order line computed numerically (figure 11). The negative slope is a consequence of the negative entropy of the spin glass solution.

6 Concluding Remarks

We have reanalyzed the replica-symmetric solution of the spin-glass model introduced by Ghatak and Sherrington (1977) by means of detailed numerical study and asymptotic calculations close to the tricritical point and at low temperatures. In the region where the model is believed to undergo a first-order phase transition, there are some difficulties not found in the Sherrington-Kirkpatrick model, such as multiple spin-glass solutions or complex eigenvalues of the stability matrix. However, it seems to be possible to describe the model within the replica-symmetric approximation without incurring in more serious inconsistencies than those already present in the standard Sherrington-Kirkpatrick model. In particular, we did not find that the free energy along the first-order transition is discontinuous, a possibility which has been mentioned by Lage and de Almeida (1982), but rather we used the continuity of the free energy to locate the first-order transition. Lage and Almeida as well as Mottishaw an Sherrington (1985) reproduce the phase diagram of Ghatak and Sherrington (Figure 1) where the propounded first-order line is located much below what we believe to be the correct position (Figures 10-11). As an argument against their first-order line, we would like to point out that the slope of their first-order line at $T = 0$ is inconsistent with a negative zero-temperature entropy of the spin-glass phase as a consequence of the Clausius-Clapeyron equation discussed in subsection 5.4. The asymptotic results of Mottishaw and Sherrington in the vicinity of the tricritical point, in particular for the first-order line, are also at variance with our results, despite the fact that the asymptotic expressions for the paramagnetic and spin-glass solutions are the same. Qualitatively, their results do not differ very much from ours, but their expressions are incompatible with the results of our numerical calculations. Although we believe our replica-symmetric solution of the Ghatak-Sherrington model to be correct, it manifests the well known pathologies already present in the Sherrington-Kirkpatrick model. The zero-temperature entropy, for example, is always negative. The instability of the replica-symmetric solution in the region of the first-order transition, on the other hand, seems to be even more serious than in the Sherrington-Kirkpatrick model because all the eigenvalues of the stability matrix become negative or complex. In this sense the Ghatak-Sherrington model poses a more stringent test for the validity of the replica-symmetry-breaking solution proposed by Parisi, and it is of considerable interest to study the properties of this solution in relation to the first-order transition. In fact, the model has already been studied in the first step of the replica-symmetry-breaking scheme of Parisi (da Costa, 1989), and it yields a solution that tends to the right direction. For example, the zero-temperature entropy is less negative, and the slope of the first-order line at $T = 0$ becomes less negative. We conjecture that, in the full Parisi solution of the model, this slope will be exactly zero. Finally, we wish to mention that the Ghatak-Sherrington model on a Cayley tree has been considered by da Costa and Salinas (1990). In the infinite coordination limit the model on the tree is described by the same equations as the replica-symmetric equations of this paper, and consequently leads to essentially the same results.

Acknowledgments

We thank J R de Almeida for useful discussions. One of us (F A C) acknowledges a doctoral fellowship from Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP). C S O Y and S R S also acknowledge partial financial support from Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

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